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Evaluation of Trace Element Release from Fluidized-Bed Combustion Systems

Westinghouse Research and Development Center, Pittsburgh, Pa

Prepared for

Industrial Environmental Research Lab, Research Triangle Park, N C

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EVALUATION OF TRACE ELEMENT RELEASE FROM FLUIDIZED-BED COMBUSTION SYSTEMS

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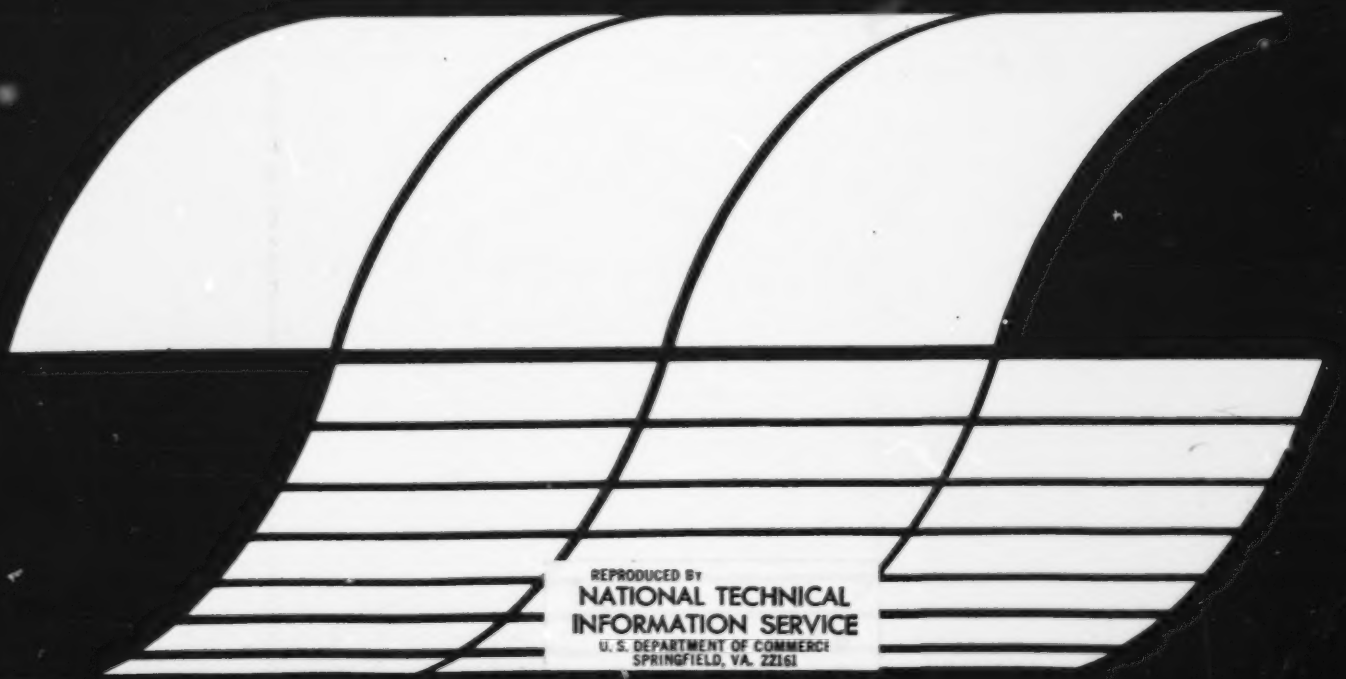

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PREFACE

The Westinghouse R&D Center is carrying out a program to provide experimental and engineering support for the development of fluidized-bed combustion systems under contract to the Industrial Environmental Research Laboratory, U.S. Environmental Protection Agency (EPA), at Research Triangle Park, NC. The contract scope includes atmospheric and pressurized fluidized-bed combustion processes as they may be applied for steam generation, electric power generation, or process heat. Specific tasks include work on calcium-based sulfur removal system studies (e.g. sorption kinetics, regeneration, attrition, modeling), alternative sulfur sorbents, nitrogen oxide emissions, particulate emissions and control, trace element emissions and control, spent sorbent and ash disposal, and systems evaluation (e.g. impact of new source performance standards on fluidized-bed combustion system design and cost).

This document contains the results of work defined and completed under the trace element task from December 1975 to January 1977. Results from work carried out by Westinghouse or reported by other investigators after January 1977 are not assimilated into this task report. The work reported represents an extension of prior work completed by Westinghouse under contract to EPA. Results from this prior work on fluidized-bed combustion include:

- Assimilation of available data on fluidized-bed combustion, including sulfur dioxide removal, sorbent regeneration, sorbent attrition, nitrogen oxide minimization, combustion efficiency, heat transfer, particle carry-over, boiler tube corrosion/erosion fouling, and gas-turbine erosion/corrosion deposition

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- Assessment of markets for industrial boilers and utility power systems
- Development of designs for fluidized-bed industrial boilers
- Development of designs for fluidized-bed combustion utility power systems: atmospheric-pressure fluidized-bed combustion boiler-combined cycle power systems, adiabatic fluidized-bed combustion-combined cycle power systems--including first- and second-generation concepts
- Preparation of a preliminary design and cost estimate for a 30 MW (equivalent) pressurized fluidized-bed combustion boiler development plant
- Assessment of the sensitivity of operating and design parameters selected for the base power plant design on plant economics
- Collection of experimental data on sulfur removal and sorbent regeneration using limestone and dolomites
- Preparation of cost and performance estimates for once-through and regenerative sulfur removal systems
- Evaluation of alternative sulfur sorbents
- Collection and analysis of data on spent sorbent disposal--utilization and environmental impact of disposal
- Projection and analysis of trace emissions from fluidized-bed combustion systems
- Analysis of particulate removal requirements and development of a particulate control system for high-temperature, high-pressure fluidized-bed combustion systems
- Construction of a high-pressure/temperature particulate control test facility
- Development of plant operation and control procedures
- Construction of a corrosion/erosion test facility for the 0.63 MW Exxon miniplant
- Continued assessment of fluidized-bed combustion power plant cycles and component designs to evaluate environmental impact.

The results of these surveys, designs, evaluations, and experimental programs provide the basis for the work being carried out under the current contract. Seven reports are available which document the prior contract work (see references 30-32). Other reports published under the current contract include "Alternatives to Calcium-Based Sorbents for Fluidized-Bed Combustion: Conceptual Evaluation,"[33] "Calcium-Based Sorbent Regeneration for Fluidized-Bed Combustion,"[34] and "Disposal of Solid Residue from Fluidized-Bed Combustion: Engineering and Laboratory Studies."[35]

ABSTRACT

The chemical fate of minor and trace elements is important in assessing the environmental impact of the fluidized-bed combustion (FBC) process and, for certain elements, in determining the potential for deposits or corrosion in process equipment. Four trace elements of environmental concern are investigated: lead, beryllium, mercury, and fluorine. Equilibrium product distributions for these elements at operating conditions corresponding to atmospheric and pressurized fluidized-bed combustion systems are projected on the basis of thermodynamic calculations. The results show which elements are likely to be volatilized in the high-temperature zone of the combustor and which are likely to condense on cooling the gases. The projections are compared with available experimental plant data. Alternatives for continuously monitoring the release of the four toxic trace elements in the laboratory were also investigated.

The thermodynamic analysis shows that essentially all the lead, mercury, fluorine, and beryllium can be volatilized in the fluidized-bed combustor. Partial beryllium and fluorine condensation in the form of clay and alkali compounds will occur. Lead condensation is affected by the chlorine available. These thermodynamic projections provide a basis for experimental and monitoring studies. Initial plant data generally confirm the projections.

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SECTION 1

INTRODUCTION

Conventional steam-turbine cycles and combined steam- and gas-turbine cycles are being utilized with fluidized-bed coal combustion techniques, (e.g., atmospheric-pressure fluidized-bed boilers, supercharged fluidized-bed boilers, and adiabatic combustors) to develop power generation systems having superior environmental control and economics. Current development programs primarily emphasize the use of calcium-based sorbents (limestones and dolomites) to provide in situ control of SO_x in the combustor.

Pilot-scale tests of fluidized-bed combustion of coal have shown that air pollution from SO_2 and NO_x emissions can be reduced to meet EPA requirements. Coal, however, contains many minor and trace elements in addition to the combustible carbon (C), hydrogen (H), and sulfur (S). In assessing the environmental impact of the fluidized-bed combustion process, it is important to determine the chemical fate of these trace elements, some of which have toxic forms at certain concentrations.

Ideally, a complete model of the process would include a knowledge of the compounds in which these elements are combined in the process feedstock. Kinetic models of the reactions that occur during coal combustion would then be used to calculate the product distribution of chemical species as a function of the process operating conditions. This would permit quantification of the concentration and type of chemical compound emitted in the solid or gaseous effluents from the plant.

Although the ranges of concentrations of many elements of interest in U.S. coals have been determined, the chemical form of each element is not always known and may vary significantly in different coals. The

kinetics of the chemical reactions occurring are not known. It is possible, however, to fall back on a common assumption used in high-temperature chemistry and assume, as a first level of approximation, that thermodynamic equilibrium will be reached in the bed and that the equilibrium product distribution will be characteristic of the process effluent.

Four trace elements of environmental concern - lead, beryllium, mercury, and fluorine - are studied. The equilibrium product distribution has been investigated for the anticipated operating ranges of different designs of fluidized-bed combustors. The data are then discussed in the light of available experimental evidence.

Of those elements known to be present in coal, lead and mercury are also among the most toxic, persistent, and abundant of the heavy metals in the environment. Coal combustion contributed 920 tons of lead (0.5 percent of total emissions) in 1968, but since the major source (gasoline combustion - 94.8 percent) has declined recently, the relative importance of potential lead emissions from the anticipated increase in coal burning has greatly increased. Inorganic mercury is readily converted to methyl mercury by microorganisms, and this compound easily enters the human food chain. Beryllium is a notoriously toxic element in all of its common inorganic forms (oxides, chlorides, sulfates), and the original air pollution limits proposed (0.01 $\mu g/m^3$) reflected this concern. Later work has shown that high-temperature-fired oxide is far less toxic. Fluorine is of concern because the ultimate product of release, fluoride salts, is readily ingested by both animals and humans, and fluorine has been responsible for serious air pollution in localized areas where emissions are high.

SECTION 2

CONCLUSIONS

Conclusions from the initial phase of the study on trace element emissions are reported. Lead, beryllium, mercury, and fluorine, four trace elements of environmental concern, were investigated.

The thermodynamic analysis shows that essentially all the fluorine, beryllium, mercury, and lead can be volatilized in the high-temperature zone of the fluid-bed combustion process. For the beryllium and fluorine species, some condensation will occur on cooling the gases. The gaseous mercury released is stable to ambient temperatures. The fate of lead is more complex and depends heavily on both the feedstock material and the operating conditions of the process. At atmospheric pressure, or for low-chlorine coals, lead is largely volatilized as lead oxide, which will condense on particulate matter on passing through the cooler parts of the system. At high pressures and with high-chlorine coals, there is a tendency for lead tetrachloride to form in the gas phase.

Continuous monitoring of the toxic trace element release from the feed materials cannot be accomplished using the flame emission spectrophotometric apparatus. To achieve this objective, alternative methods and high-temperature sampling techniques have to be developed. A reasonable approach may be the determination of the total trace element release (vapor and entrained particulates) through an analysis of condensates collected at selected time intervals, using spark source mass spectroscopic and neutron activation techniques.

SECTION 3

RECOMMENDATIONS

- Thermodynamic projections have resulted in three results that correlate very well with experience (those concerning the emission of volatile PbO, Hg, and HF), one result for which there is some evidence (volatile loss of Be), and one result that is surprising - loss of lead as $PbCl_4$ in pressurized fluidized-bed combustors. This last finding should be tested by analyzing solid effluents from the Exxon miniplant to see if depletion of lead is observed at high pressures. In addition, laboratory experiments on the effect of partial pressure on retention of lead in fluidized-bed coal combustor ash at pressure and temperature (10 atm, 43 K) should be carried out.
- A comparison should be made of the results of thermodynamic projections using the Westinghouse programs and those available from other sources, to search for inconsistencies and for a firmer data base.
- The projections will be extended to include other potentially volatile elements present in coal - e.g., vanadium - and other elements that may act as getters for volatile elements, such as boron, or aluminosilicates.

SECTION 4

FEEDSTOCK TRACE ELEMENTS

COAL

Intensive efforts, largely sponsored by EPA, have been directed at determining the trace element composition of U.S. coals. Work in this area has been reviewed by Magee,[1] and the available data show a consensus of the expected concentrations of elements of interest. The concentrations of the four elements chosen for study are shown in Table 1. There has been much dispute about the level of mercury, Hg, in coal and its emission from coal-fired power plants.

Concern about mercury in coals has been exaggerated by two facts. Joensuu[2] concluded that 3000 Mg of mercury were released annually, worldwide, from coal combustion, an amount comparable to that resulting from industrial use of mercury, 10,000 Mg. Second, apparently high values for mercury in coal were published by Headlee and Hunter,[3] of the West Virginia Geological Survey.

According to Magee, however, Joensuus's 3000 Mg estimate is based on an assumed value of 1 ppm mercury in coal: the true value of 0.18 ppm yields 540 Mg total release, more than an order of magnitude less than the industrial pollution value. In addition, the Headlee and Hunter high values are reputed to be the result of a typographical error.

Two sets of analyses confirm the level of mercury in coal to be as stated by Magee: Gluskoter[4] found 0.20 ± 0.20 ppm mercury in 102 U.S. coals; Page,[5] et al. found 0.11 ± 0.06 ppm mercury in

TABLE 1. TRACE ELEMENTS IN COAL

Magee (1973) [Review of Literature][2]		Gluskoter (1973) 101 Samples[4] (ppm)	Westinghouse (1973) 24 Samples Western Coals[5] (ppm)
Hg	0.18	0.20 ± 0.2	0.11 ± 0.06
F	50-160	60.94 ± 20.99	61.25 ± 31.99
Be	0.64-3.1	1.61 ± 0.82	1.43 ± 2.13
Pb	4-14	34.8 ± 43.7	24.2 ± 13.5

western coals; the U.S.G.S. found 0.06 ppm for the same area.[1] The values reported by Gluskoter for fluorine, F, beryllium, Be, mercury and lead, Pb, were used in the calculations reported here.

It has been noted that the low concentration of fluorine in coal shows it to be depleted, relative to its concentration in the earth's crust, by one order of magnitude; agreement on its concentration in U.S. coals by different schools of analysts is relatively good. For beryllium, agreement among the analysts is excellent. Gluskoter's values for lead are higher than those reported in the other studies.[4]

In order to carry out thermodynamic projections of trace element release, it was necessary to include in the analyses other elements, such as chlorine, Cl, which can act as an anion carrier for metals. These values are all taken from Gluskoter's work(see Table 3).[4]

LIMESTONES AND DOLOMITES

There is no recent study of trace element concentrations and their distribution in limestone and dolomite. Estimates of the maximum likely concentrations are made possible for some elements by atomic emission data (within a factor of three) and from neutron activation analysis data obtained by Exxon[6] and Argonne National Laboratories (ANL).[7] Several of the Westinghouse limestone or dolomite analyses are shown in Table 2. It should be noted that these techniques do not determine the fluorine or mercury content of a given sample.

Upper limits to the concentrations of two elements were obtained from an unpublished study by the Ohio State Geological Survey[8] on the concentration of trace elements in dolomites from that state. Analysis of nine typical U.S. limestones and dolomites reported by Harvey[9] were found at the conclusion of this work: they show a mean value for mercury of 0.07 ppm ± 0.07, indicating that the choice of 0.16 ppm mercury in the sorbent was conservatively high.

The trace element concentrations in the sorbent (a dolomite) assumed for this study are shown in Table 3. The number of dolomites

TABLE 2. ANALYSIS BY EMISSION SPECTROSCOPY OF TRACE IMPURITIES IN SELECTED U. S. LIMESTONES AND DOLOMITES, WT %

	No. 10 Glasshouse 1337 (Ohio: Dolomite)[10]	Tymochtee (Ohio: Dolomite)[10]	CP&L (Texas: Limestone)[11]
Al	0.1	>0.4	0.4
Ag	<0.0001	<0.0001	<0.0004
B	<0.0004	0.008	<0.004
Ba	—	—	0.0004
Be	—	—	<0.0004
Bi	<0.0004	<0.0004	<0.0004
Cd	<0.04	<0.04	<0.04
Co	<0.004	<0.004	<0.0004
Cr	<0.004	<0.004	<0.004
Cu	<0.0004	0.001	0.008
Fe	0.04	0.1	0.2
K*	0.0250	0.3700	0.116
Li	—	—	<0.0004
Mn	0.004	0.004	0.04
Mo	<0.004	<0.002	<0.004
Na*	0.0180	0.0329	0.014
Nb	<0.004	<0.004	<0.004
Ni	<0.0004	<0.0004	<0.004
P	—	—	<0.004
Pb	<0.004	<0.004	<0.0004
Sb	<0.004	<0.004	<0.004
Si	0.3	2.	~2.
Sn	<0.002	<0.002	<0.004
Sr	—	—	0.08
Ti	0.002	0.008	0.04
V	<0.004	<0.004	<0.004
Zn	0.02	<0.02	<0.004
Zr	<0.02	<0.004	<0.004

*Atomic absorption

TABLE 3. COAL AND SORBENT COMPOSITION

Coal Composition for Fluid-Bed Combustor[4]		
Element	wt%	2σ wt%
C	70.28	
H	4.95	
N	1.30	
O	8.68	
S	3.27	
Cl	0.14	0.28
K	0.16	0.22
Na	0.05	0.09
F*	60.94	81.93
Be*	1.61	2.43
Hg*	0.20	0.40
Pb*	34.78	78.47

Sorbent (Dolomite) Composition for Fluid-Bed Combustor[10,12]	
C	13.031
H	--
N	--
O	52.06
S	--
Cl*	2000, 806, 200
K*	4000, 300, 100
Na*	300, 150, 50
F*	10
Be*	4
Hg*	0.16
Pb*	18.5
Ca	21.70
Mg	13.19

*Value in ppm

for which minor and trace element data are available is small, and it is not possible to represent the spread of the likely values, as in the Gluskoter study, on coal. Therefore, values representing the highest and lowest alkali and chlorine content were selected.

SECTION 5

THERMODYNAMIC PROJECTIONS

APPROACH

Thermodynamic Calculation Basis

The feedstock chosen in the trace element fluid-bed combustor study is a model coal that has the mean composition of U.S. coals found by Gluskoter (Table 3).[4] The minor (chlorine, sodium, Na, potassium, K,) and trace (fluorine, beryllium, mercury, lead) element constituents of the coal are varied as:

1. The mean value (referred to as the "mean coal" or "mean sorbent")
2. The mean value + (2 σ) (referred to as the "high or low coal", or "high or low sorbent")

where σ = standard deviation of the concentration determined by Gluskoter for 101 U.S. coals.

The impact of the desulfurizing sorbent is projected by using three levels of chlorine, three levels of alkali (sodium and potassium), and the four trace elements at their mean values (Table 3).

Each projection is calculated at equilibrium in 10, 100, and 300 percent excess air, from 1 to 15 atmospheres, and from 300 to 1200 K. The excess air values and the system pressures were selected to cover the range expected in the alternative variations of the fluidized-bed combustion process. The temperatures were selected to cover the range that would be seen by the combustion gases, from the combustion zone of the furnace through the ducting to the exhaust stack.

Each projection is carried out for a 4 percent sulfur coal with a steady-state SO_x value in the effluent corresponding to 0, 90, and 99 percent sulfur removal.

Table 4 indicates the moles of each key element fed into the bed per 100 g of coal burned, based upon the composition indicated in Table 3.

Equilibrium Calculations

The equilibrium composition for trace element fluid-bed combustion conditions is calculated[12] by minimizing the Gibbs free energy of the polyphase system, using the techniques of Geometric Programming,[13] in addition to satisfying the mass conservation equations.

The Gibbs free energy (G) of a multicomponent system is represented by a summation over the mixture chemical species, i.e.,

$$G = \sum_i n_i G_i \ , \tag{1}$$

where $G_i = \mu_i$ is the molar chemical potential and n_i is the number of moles of the i^{th} species. The molar chemical potential is expressed as

$$\mu_i = \mu_i^o + \delta \ (RT \ln P_i) \ , \tag{2}$$

where for a gaseous species $\delta = 1.0$, and for a condensed species $\delta = 0$. In the above equation P_i is the partial pressure of the gaseous species, T is the gas temperature, R is the universal gas constant, and μ_i^o is the species' chemical potential at unit fugacity,

$$\mu_i^o = H_i^o - TS_i^o \ , \tag{3}$$

TABLE 4. MOLES OF KEY ELEMENTS FED TO THE FLUID-BED PER 100g OF COAL BURNED

Element		System		
		High Coal-High Sorbent	Mean Coal-Mean Sorbent	Mean Coal-Low Sorbent
C		6.1563 moles	6.1563 moles	6.1563 moles
H		4.9107	4.9107	4.9107
N	(a)	57.41855	57.41855	57.41855
	(b)	104.39774	104.39774	104.39774
	(c)	208.79473	208.79473	208.79473
O	(a)	16.70376	16.70376	16.70376
	(b)	29.1919	29.1919	29.1919
	(c)	56.9430	56.9430	56.9430
S	(d)	0.124800	0.124800	0.124800
	(e)	0.012480	0.012480	0.012480
	(f)	0.001248	0.001248	0.001248
Cl		9.455E-3	4.5765E-3	4.1047E-3
K		8.4505E-3	4.3038E-3	4.1627E-3
Na		4.3108E-3	2.578E-3	2.234926E-3
F		4.4572E-4	3.3526E-4	3.3526E-4
Be		3.921E-5	3.012E-5	3.012E-5
Hg		2.016E-7	1.019E-7	1.019E-7
Pb		4.033E-5	1.92505E-5	1.92505E-5

NOTE: Excess air = 10%(a), 100%(b), 300%(c). Sulfur removal for dolomite in this study uses a Ca/S ratio of 1.25/1 for 0% removal (d), 90% removal (e), and 99% removal (f). The impact of Ca/S ratio on the trace metals fed via the dolomite has not been considered.

where H_i^o (molar enthalpy) and S_i^o (molar entropy) are the species' standard thermochemical properties, which are functions of the species standard specific heat, $C_{P,i}^o$, i.e.,

$$H_i^o(T) = \int_{T_r}^{T_o} C_{P,i}^o \, dT + \Delta H_f^o(T_r) \tag{4}$$

and

$$S_i(T) = \int_{o}^{T} \frac{C_{P,i}^o \, dT}{T} , \tag{5}$$

where ΔH_f^o is the standard heat of formation for the compound at the reference temperature (T_r) of 298.15 K.

The chemical equilibrium program determines the value of n_i for each species in all possible solid, liquid, or gaseous phases, given the species' standard thermochemical data (as reported in the literature),[15-23] the total gas pressure, and the mass constraints on the system. Tables 5 and 6 illustrate the species for which thermochemical data are presently available for use in the current computer study. The data for each species have been reduced (see Program *FJANAF) and used as input for the chemical equilibrium calculations. The reaction of fluorine with combustion gases, for example, uses compounds formed from carbon, C; hydrogen, H; nitrogen, N; oxygen, O; sulfur, S; chlorine, and fluorine. The interaction of alkali with fluorine additionally requires specification of those compounds containing those same elements and associated alkali compounds. Table 7 lists the computer programs used in calculating the equilibrium composition and thermochemical properties of the fluid-bed combustion mixture at defined parameters of pressure and temperature for a given system defined by the considered elements. Additional CALCOMP routines are available for visually displaying the data as either profile or isometric plots.

Multiple reactions that occur in fluid-bed combustors produce numerous solids, liquids, or gaseous compounds that are dependent on the

TABLE 5. C-H-N-O-S-Cl-K-Na SPECIES CONSIDERED IN FLUID-BED COMBUSTION REACTIONS

Gases			Solids/Liquids
C	COS	NO_2*	C
CCl	Cl*	NO_3	K
CCl_2	ClHO*	NS	KCl
CCl_2O	ClO*	N_2*	K_2CO_3
CCl_3	ClO_2	N_2H_2	KCN
CCl_4	Cl_2*	N_2H_4	KH
CH	Cl_2O	N_2O*	KOH
CHN	H	N_2O_3	KO_2
CHNO	HCl*	N_2O_4	K_2Cl_2
CHO	HK	N_2O_5	$K_2O_2H_2$
CH_2	HNO	Na*	K_2O
CH_2O	HNO_3*	NaCl*	K_2O_2
CH_3	HO*	NaCN	K_2SO_4*
CH_4	HO_2	NaH	Na
CN	HS	NaO	NaCl
CHN	H_2*	NaOH*	$NaCO_3$
CN_2	H_2O*	Na_2	NaCN
CO*	H_2S	Na_2Cl_2*	NaH
CO_2*	H_2SO_4*	$Na_2C_2N_2$	NaOH
C_2	K*	$Na_2O_2H_2$*	NaO
C_2Cl_4	KCl*	Na_2SO_4*	Na_2Cl_2
C_2Cl_6	KCN	O*	$Na_2O_2H_2$
C_2H	KO	O_2*	Na_2S
C_2H_2	KOH*	O_3	Na_2SO_4*
C_2H_4	K_2	S	
C_2H_4O	K_2Cl_2*	S_2	
C_2N	$K_2C_2N_2$	S_3	
C_2N_2	$K_2O_2H_2$*	S_8	
C_2O	K_2SO_4*	SO	
C_3	N	SO_2*	
C_3O_2	NH	SO_3*	
C_4	NH_2	S_2O	
C_4N_2	NH_3		
CS	NO*		

*Species resulting in fluid-bed combustion conditions for C-H-N-O-S-Cl-K-Na Systems as projected by the CHEMEQ *INITAL program.

TABLE 6. TRACE SPECIES CONSIDERED IN FLUID-BED COMBUSTION REACTIONS

Gases			Solids/Liquids
CF	F_2N	BeC_2	FK
CFO	F_2N_2	BeCl	FNa
CFN	F_2Na_2	$BeCl_2$	F_2HK
CF_2	F_2O	Be_2Cl_4	
CF_2O	F_2OS	BeH	Hg
CF_3	F_2O_2S*	BeH_2	HgCl
CF_4	F_3Cl	BeN	$HgCl_2$
CF_4O	F_3N	BeO	Hg_2Cl_2
$CHClF_2$	F_3NO	Be(OH)2*	HgO
$CHCl_2F$	F_4N_2	Be_2O	
CHFO	F_5Cl	Be_2O_2	Pb
CHF_3	HF*		$PbCO_3$
CH_2ClF	SF	FHg	PbCl
CH_2F_2	SF_2	F_2Hg	PbO
C_2F_3N	SF_3		PbO_2
C_2HF	SF_4	PbF	Pb_3O_4
CC1FO	SF_5	PbF_2	PbS
$CC1F_3$	SF_6	PbF_4	$PbSO_4$
CCl_2F_2	Hg*		$PbO \cdot PbSO_4$
CCl_3F	Hg_2*		$2PbO \cdot PbSO_4$
F	HgCl*		$4PbO \cdot PbSO_4$
FCl	$HgCl_2$*		
FHO	HgH*		Be
FK*	HgO*		$BeCl_2$
FNa*			BeO
FN	Pb		BeSO4*
FNO	Pb_2		Be_2C
FNO_2	PbCl*		Be_3N_2
FNO_3	$PbCl_2$*		
FO	$PbCl_4$*		F_2Hg
FO_2	PbH		F_2Hg_2
F_2	PbO*		
F_2K_2			PbF_2

*Trace species found to result at fluid-bed combustion conditions, based upon the thermodynamic projection model.

TABLE 7. CHEMICAL EQUILIBRIUM COMPUTER PROGRAMS[13]

CHEMEQ* FJANAF	Program designed to curve-fit the thermochemical data ($\Delta H^{\circ}_{f298.15}$, $S^{\circ}_{298.15}$) of compounds as a function of C_p for solids and liquids, and in terms of the molecular constants for gases.
CHEMEQ* INITAL	Program designed to select the specific (active) compounds that are involved in the reactions at equilibrium. For example, 175 compounds are included in the INITAL calculation that are considered as possible candidate species for the reaction. The results of INITAL indicate that only 48 react as either major or trace constituents. The reduction in the number of compounds involved in the equilibrium reaction is now within the limits of the CHEMEQ* GASF program.
CHEMEQ* GASF	Program designed to calculate the number of moles, mole fraction, pressure, part/cc, density, and mass of the compounds contained in the mixture at equilibrium as a function of pressure and temperature for specified element concentrations. Modifications to GASF include the options for the creation of the COFILE, which enables the user to plot the partial pressure of the gas and the number of moles of solid/liquid formed as a function of temperature. COFILE can be expanded to include a series of calculations at various pressures, from which isometric plots may be generated.
CHEMEQ* THERMO	Program designed to calculate the thermochemical properties of the equilibrium mixture at defined pressures and temperatures.

pressure and temperature of the system. The final concentration of each phase is a function of the relative concentration of specific elements or compounds introduced into the reaction as constituents of coal and/or sulfur sorbents. For example, the sulfur concentration of coal defines the level at which SO_3, SO_2, and alkali sulfates are formed. With the addition of the calcium-based sorbents, the initial sulfur levels are reduced. Furthermore, a high level of chlorine has been shown to suppress the formation of liquid/solid alkali sulfates to lower temperatures. Chlorine present in fluid-bed gases reacts with the trace elements of coal or sorbent that are released into the effluent gases, producing gaseous trace chlorides. Silicon, Si, and aluminum, Al, the major clay constituents of coal, react with alkali and trace elements, forming complex structures that are removed as solids in the waste and spent sorbent process. A composite diagram (Figure 1) illustrates those reactions that are projected to result, according to the thermodynamic calculations, when trace elements are present in fluid-bed combustion gases.

In order to illustrate the projected major reactions of the trace elements, the partial pressure of the gaseous trace compounds and the number of moles of trace solids produced at 10 atmospheres are plotted in Figure 2 as a function of temperature for fluid-bed operating conditions at 10 percent excess air with 90 percent sulfur removal and with the highest anticipated trace concentrations (high coal-high dolomite). The calculated equilibrium partial pressures for the phase diagram are tabulated in Appendix A. Reference to this section provides useful information about the modification required on the phase diagram for systems operating at pressures other than 10 atm. At fluid-bed combustion temperatures only gaseous trace compounds are projected to form. Trace solids are predicted to be thermochemically unstable at elevated operating temperatures. As shown in Figure 2, the solid $BeSO_4$ is projected to form at temperatures below 600 K for fluid-bed systems containing carbon, hydrogen, nitrogen, oxygen, sulfur, chlorine, fluorine, beryllium, mercury, and lead. The thermodynamic calculations, however,

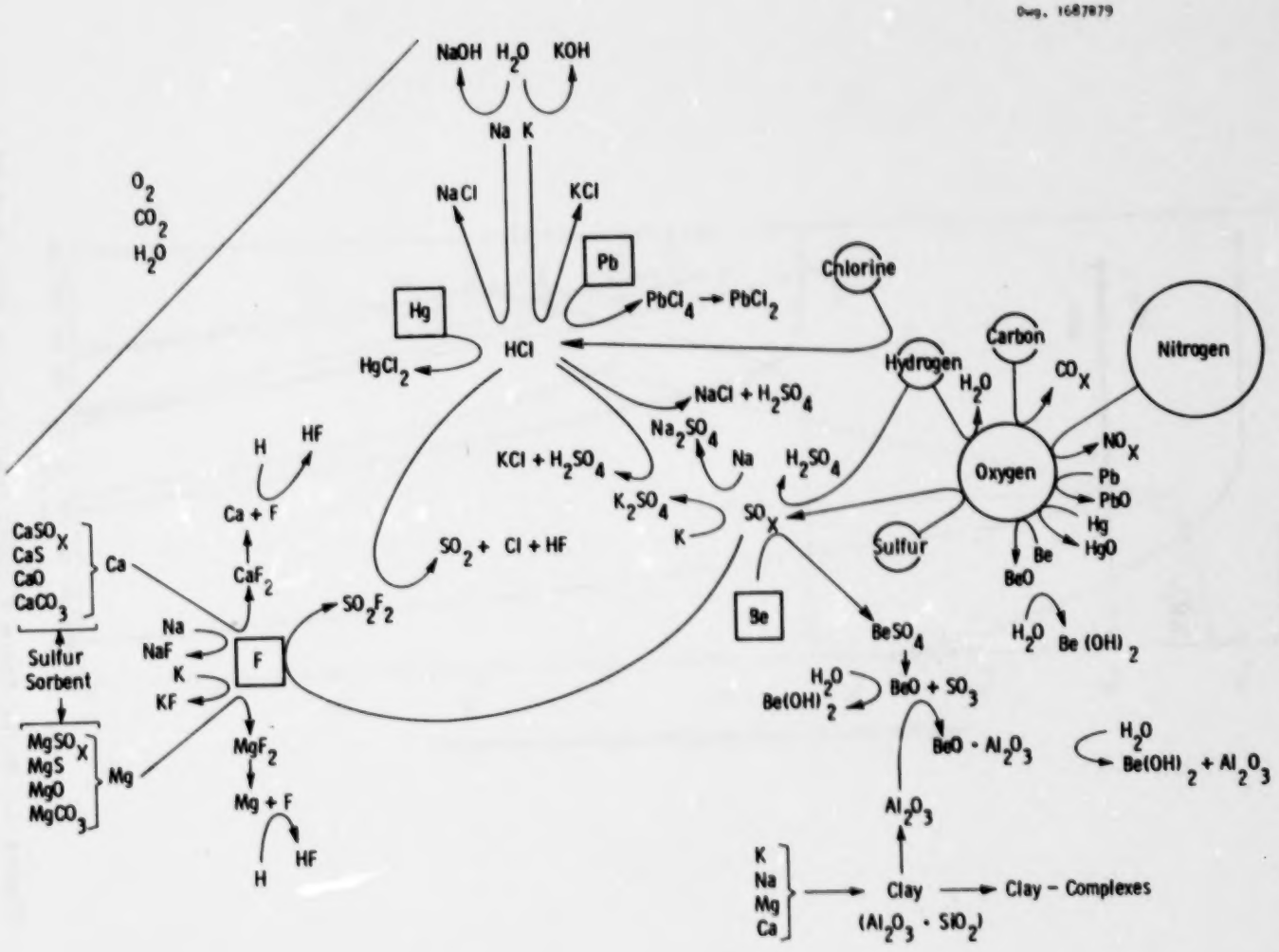

Figure 1. Possible Reaction Pathways in the Trace Element System.

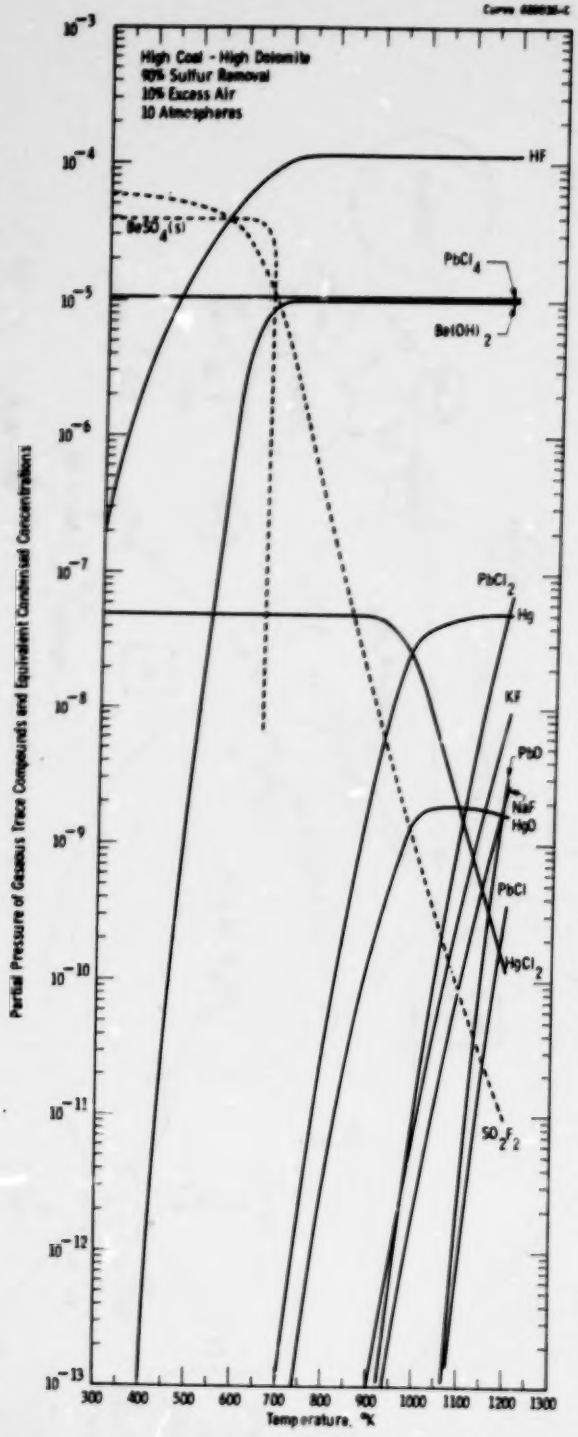

Figure 2. Major Trace Element Reactions for High Coal-High Dolomite Systems at 10 Atmospheres Total Pressure as a Function of Temperature.

assumed that all the elements in coal and sorbent were "matrix free." If some elements in the feed materials were instead "matrix bound," the elements would be less capable of reactions, and the concentrations of gaseous products would be lower than those projected here.* Fluorine and beryllium, for example, may exist as calcium or magnesium fluoride, CaF_2 and MgF_2, and as beryllium aluminate, $BeO \cdot Al_2O_3$, in the feed material. Unless total combustion of the coal and dolomite has occurred, the projected levels of both volatile and condensed phases should be regarded as the maximum trace concentrations at any location in the system.

It should be noted that this study considers only the reactions of compounds for which thermodynamic data are available. It is reasonable to assume that other compounds may form in the fluid-bed system. Data for such compounds have not been cited in the literature, however, nor have estimates of their free energy, heats of formation, or molecular constants been made. It is the opinion of the authors that compounds not reported in the literature are less likely to form than are those for which data are cited.

THERMODYNAMIC STABILITY OF THE TRACE ELEMENT SPECIES

Fluorine

At the highest temperatures, in the range of 1100 to 1200 K, fluorine is projected to be released to the gas phase as NaF(g), sodium fluoride; KF(g), potassium fluoride; and HF(g), hydrogen fluoride, the preponderant fluorine species. As the temperature falls toward 800 K, the HF recombines with the excess calcium oxide to form solid CaF_2; and at lower temperatures (below 700 K) solid MgF_2 is the stable compound. At low temperatures, 300 to 500 K, sulfuryl difluoride, SO_2F_2, is the equilibrium gaseous product, even with 90 percent sulfur

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*Matrix bound - Element entrapped with a solid structure not permitted to react further with surrounding gases.
Matrix free - Element reactive with a solid structure capable of reacting simultaneously with the surrounding gases.

removal. In systems that consider the formation of calcium and magnesium fluorides, the formation of gaseous sulfuryl difluoride is suppressed.

As the concentration of sulfur in the fluidized-bed combustor effluent gas is decreased, the production of gaseous SO_2F_2 is reduced. At the lower gas phase sulfur concentrations fluorine that remains in the gas phase combines instead with either hydrogen, sodium, or potassium, forming gaseous HF or alkali fluorides instead of SO_2F_2.

In the presence of HCl formed in the combustion gases, SO_2F_2 is converted to HF, as shown by the following reaction:

$$SO_2F_2(g) + HCl(g) \rightleftharpoons SO_2(g) + Cl_2(g) + HF(g) \quad . \qquad (6)$$

This reaction is governed not only by the level at which fluorine, sulfur, and chlorine are present, but is a function of the temperature and pressure of the reaction. At low temperatures (300 to 500 K) the major compound formed is SO_2F_2; as the temperature increases, the reaction is pushed to the right, favoring the formation of gaseous HF.

Reducing the sulfur concentration to levels present in 99 percent sulfur removal conditions no longer produces gaseous SO_2F_2 but, between 300 and 800 K, solid NaF. Since fluorine is bound in the form of NaF(s) at low temperatures, the projected level of HF in the gas is lowered in systems that favor total sulfur removal. At elevated temperatures HCl, formed in the combustion process, reacts with NaF, converting the alkali fluoride into the stable NaCl solid plus gaseous HF. Thus,

$$NaF(s) + HCl(g) \rightleftharpoons NaCl(s) + HF(g) \quad . \qquad (7)$$

The production of gaseous alkali fluorides occurs in both 0 and 90 percent sulfur removal systems. Lowering the concentration of sulfur increases the level of fluorine that reacts with the alkalis present in the gas phase. Equilibrium calculations indicate significant differences in the partial pressures of the alkali fluorides at low temperatures. For example, the partial pressure of $NaF_2(g)$ at 600 K is

0% S removal - 2.19×10^{-25} atm

99% S removal - 5.39×10^{-17} atm

when the total pressure of the system is 15 atmospheres. This effect is also demonstrated by the partial pressure of KF_2 gas.

Dimeric forms of the alkali fluoride (K_2F_2, Na_2F_2) result when the concentration of sulfur is further reduced to 99 percent sulfur removal conditions. The concentrations of the dimers are below those of the resulting alkali fluorides by a factor of 10^2 at 1200 K. Tables 1 through 4 of Appendix A show the partial pressures calculated at equilibrium for the most significant trace-fluorine compounds as a function of pressure and temperature. Parameters for the high coal-high dolomite system include 10, 100, and 300 percent levels of excess air at 90 percent sulfur removal conditions.

The previous discussion illustrates the reactions that occur when fluorine reacts with fluid-bed combustor gases. Consideration must be given, however, to reactions that are likely to result when limestone ($CaCO_3$) or dolomite ($CaCO_3 \cdot MgCO_3$) is present in the equilibrium system. The major reaction of fluorine with calcium and magnesium is the initial formation of solid MgF_2, which is converted to solid CaF_2, between 660 and 680 K. Calcium fluoride remains stable until 900 to 920 K but is removed at elevated temperatures, permitting the formation of HF in the gas phase. The difference between the two reaction systems may be written as:

Without carbonates

$$SO_2F_2(g) + 2HCl(g) \xrightarrow{<700\ K} SO_2(g) + Cl_2(g) + 2HF(g) \qquad (8)$$

With carbonates

$$CaF_2(s) + H_2O(g) \xrightarrow{<900\text{-}920\ K} CaO(s) + 2\ HF(g)\ . \qquad (9)$$

Introduction of the carbonate material diminishes the production of gaseous SO_2F_2 at equilibrium conditions, with fluorine re-forming as part of the CaF_2-sorbent that is removed in the spent sorbent waste process.

The major fraction of the remaining fluorine is found in the gaseous phase as HF. Both reactions 8 and 9 favor the production of HF at elevated temperatures and are unaffected by the level of sulfur present at 1000 to 1300 K. Figures 3 through 7 illustrate, for the reactions in a C-H-N-O-S-Cl-K-Na-Ca-Mg-F system, the effect pressure and temperature have on the formation of solid and gaseous fluorine compounds resulting from U.S. mean coal-mean dolomite in 90 percent sulfur removal/100 percent excess air systems.

Beryllium

As shown in Figure 2, the major gaseous beryllium species formed at high temperature is beryllium hydroxide, $Be(OH)_2$. The major gaseous sulfur species in fluid-bed combustion systems at low temperatures is H_2SO_4. As temperature increases, the H_2SO_4 vapor dissociates, forming gaseous sulfur trioxide, SO_3, and H_2O. Sufficient sulfur is present in both 0 and 90 percent sulfur removal systems to produce solid beryllium sulfate, $BeSO_4$, at temperatures of 300 to 500 K, and pressures between 1 and 15 atmospheres:

$$Be(s) + 1/2\ O_2(g) + SO_3(g) \longrightarrow BeSO_4(s)\ . \qquad (10)$$

At temperatures greater than 500 K $BeSO_4(s)$ dissociates forming solid beryllium oxide, BeO, and gaseous SO_3:

$$BeSO_4(s) \xrightarrow{(500\text{-}600\ K)} BeO(s) + SO_3(g)\ . \qquad (11)$$

The highly volatile beryllia in the fluid-bed combustion systems then react with water vapor, forming the stable gaseous $Be(OH)_2$ phase at higher temperatures:

$$BeO(s) + H_2O(g) \longrightarrow Be(OH)_2(g)\ . \qquad (12)$$

Thermodynamic calculations do not project the presence of BeO when processes are operated at 0 to 90 percent sulfur removal because of the simultaneous conversion of the $BeSO_4(s) \xrightarrow{H2O(g)} Be(OH)_2(g)$.

System: C-H-N-O-S-Cl-K-Na-Ca-Mg-F

Species Name MgF_2: Number of Moles

TEMP. (K)

	.1500+02 atm	.1000+02 atm	.5000+01 atm	.1000+01 atm
.3000+03	.2229-03	.2229-03	.2229-03	.2229-03
.4000+03	.2229-03	.2229-03	.2229-03	.2229-03
.5000+03	.2228-03	.2228-03	.2228-03	.2228-03
.6000+03	.2221-03	.2219-03	.2216-03	.2200-03
.7000+03	.0000	.0000	.0000	.0000
.8000+03	.0000	.0000	.0000	.0000
.9000+03	.0000	.0000	.0000	.0000
.1000+04	.0000	.0000	.0000	.0000
.1100+04	.0000	.0000	.0000	.0000
.1200+04	.0000	.0000	.0000	.0000

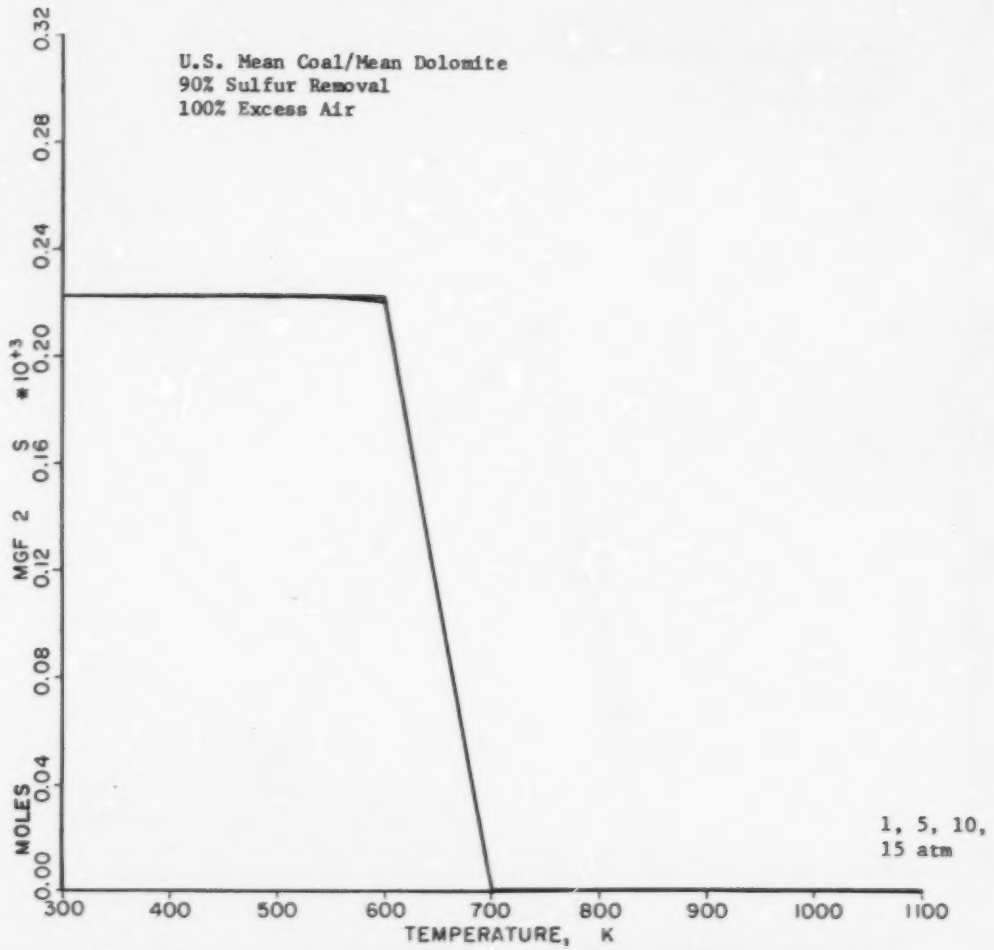

Figure 3. Number of Moles of Solid MgF_2 as a Function of Temperature and Pressure.

System: C-H-N-O-S-Cl-K-Na-Ca-Mg-F

Species Name CaF_2: Number of Moles

TEMP. (K)	.1500+02 atm	.1000+02 atm	.5000+01 atm	.1000+01atm
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.0000	.0000	.0000	.0000
.6000+03	.0000	.0000	.0000	.0000
.7000+03	.2069-03	.2069-03	.2069-03	.2069-03
.8000+03	.1681-03	.1681-03	.1681-03	.1681-03
.9000+03	.7981-04	.7980-04	.7977-04	.7967-04
.1000+04	.0000	.0000	.0000	.0000
.1100+04	.0000	.0000	.0000	.0000
.1200+04	.0000	.0000	.0000	.0000

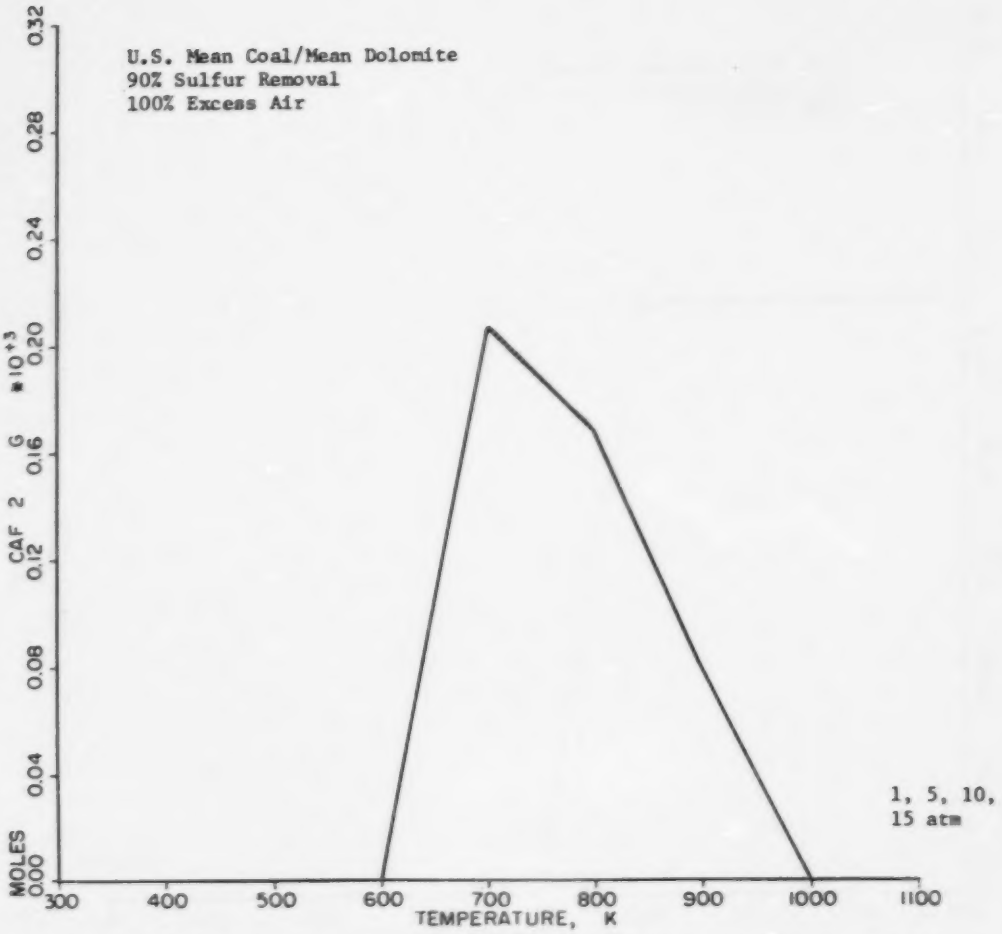

Figure 4. Number of Moles of Solid CaF_2 as a Function of Temperature and Pressure.

System: C-H-N-O-S-Cl-K-Na-Ca-Mg-F

Species Name HF: Partial Pressure

TEMP. (K)

	.1500+02 atm	.1000+02 atm	.5000+01 atm	.1000+01 atm
.3000+03	.1478-11	.9850-12	.4925-12	.9678-13
.4000+03	.6312-09	.4208-09	.2104-09	.4208-10
.5000+03	.2436-07	.1624-07	.8118-08	.1623-08
.6000+03	.3304-06	.2658-06	.1908-06	.8531-07
.7000+03	.7080-05	.4720-05	.2360-05	.4720-06
.8000+03	.2426-04	.1617-04	.8087-05	.1618-05
.9000+03	.6338-04	.4225-04	.2113-04	.4228-05
.1000+04	.9870-04	.6579-04	.3287-04	.6538-05
.1100+04	.9838-04	.6548-04	.3257-04	.6424-05
.1200+04	.9710-04	.6426-04	.3187-04	.6169-05

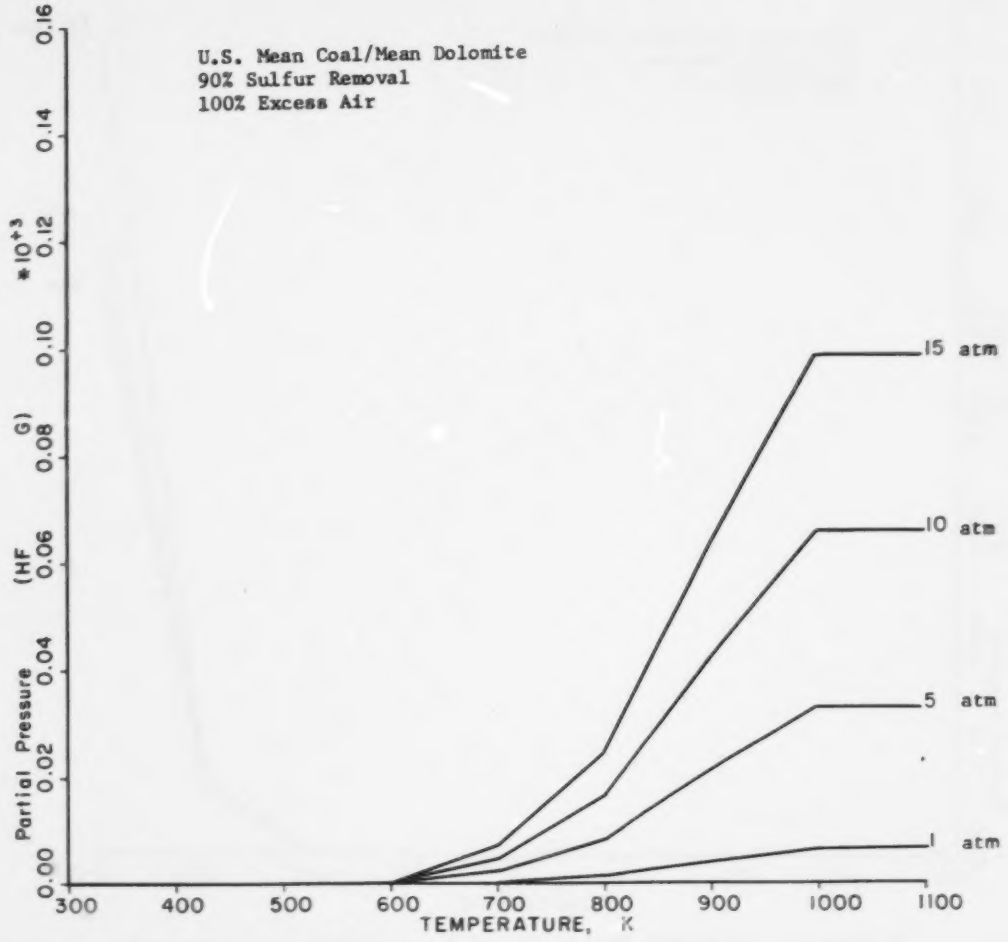

Figure 5. Partial Pressure of Gaseous HF as a Function of Temperature and Pressure.

System: C-H-N-O-S-Cl-K-Na-Ca-Mg-F

Species Name NaF: Partial Pressure

TEMP. (K)	.1500+02 atm	.1000+02 atm	.5000+01 atm	.1000+01 atm
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.2508-31	.2508-31	.2508-31	.2508-31
.5000+03	.1958-23	.1858-23	.1958-23	.1858-23
.6000+03	.2991-18	.3664-18	.5181-18	.1159-17
.7000+03	.4624-14	.4624-14	.4624-14	.4624-14
.8000+03	.2076-11	.2076-11	.2076-11	.2076-11
.9000+03	.2299-09	.2300-09	.2300-09	.2300-09
.1000+04	.6927-08	.6926-08	.6920-08	.6138-08
.1100+04	.7593-07	.7581-07	.5954-07	.5303-07
.1200+04	.3253-06	.5317-06	.3509-06	.1288-06

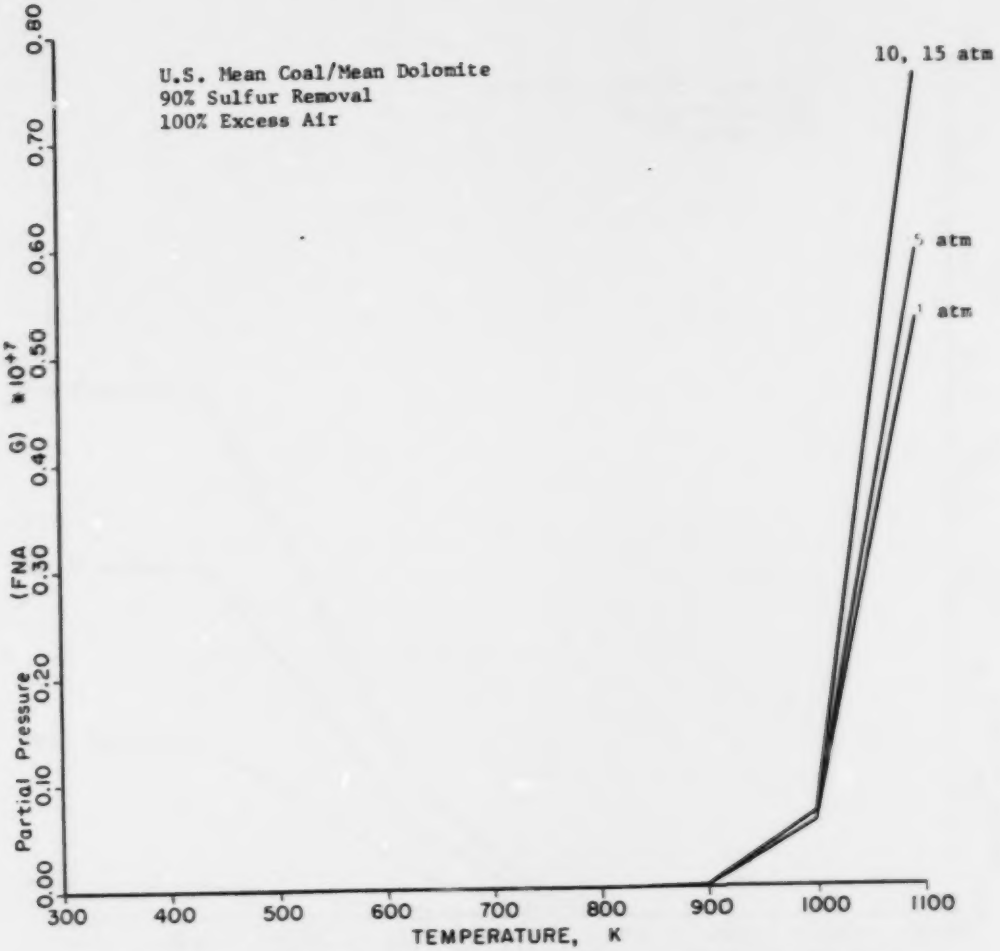

Figure 6. Partial Pressure of Gaseous NaF as a Function of Temperature and Pressure.

System: C-H-N-O-S-Cl-K-Na-Ca-Mg-F

Species Name KF: Partial Pressure

TEMP. (K)

	.1500+02 atm	.1000+02 atm	.5000+01 atm	.1000+01 atm
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.4550-30	.4550-30	.4550-30	.4550-30
.5000+03	.1715-22	.1715-22	.1715-22	.1715-22
.6000+03	.2048-17	.2508-17	.3547-17	.7930-17
.7000+03	.2695-13	.2695-13	.2695-13	.2695-13
.8000+03	.1072-10	.1072-10	.1072-10	.1072-10
.9000+03	.1021-08	.1021-08	.1021-08	.1021-08
.1000+04	.2678-07	.2677-07	.2675-07	.2373-07
.1100+04	.2633-06	.2625-06	.2065-06	.9105-07
.1200+04	.1095-05	.8878-06	.6226-06	.2695-06

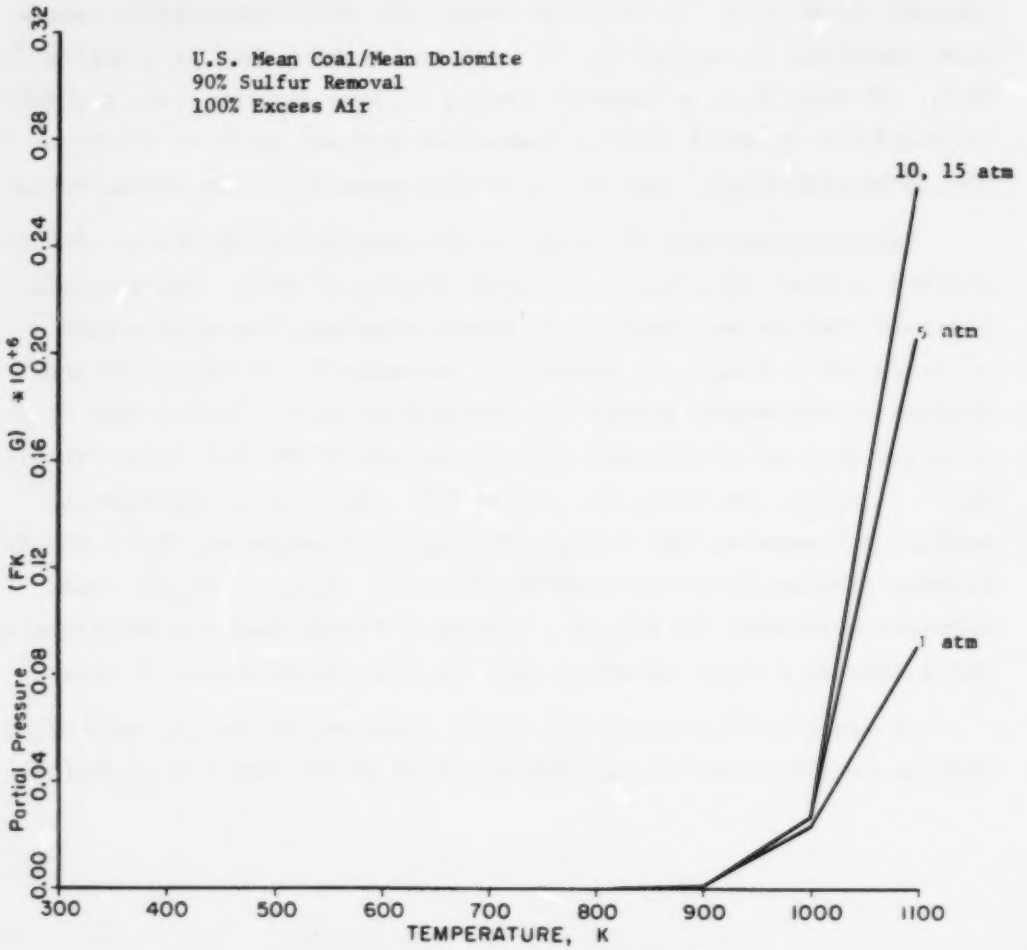

Figure 7. Partial Pressure of Gaseous KF as a Function of Temperature and Pressure.

Reduction of the sulfur concentration to the levels present at 99 percent removal no longer produces solid $BeSO_4$ but BeO(s):

$$Be(s) + 1/2\ O_2(g) \longrightarrow BeO(s) \quad , \qquad (13)$$

which reacts with water vapor to form gaseous $Be(OH)_2$. Therefore, the production of $Be(OH)_2(g)$ is enhanced at lowered temperatures when the sulfur level is reduced. Tables 5 and 6 of Appendix A list the partial pressure of $Be(OH)_2$ and the number of moles of solid $BeSO_4$ projected to result at equilibrium for fluid-bed combustor systems operating at 10, 100, and 300 percent levels of excess air and at 90 percent sulfur removal conditions. It is to be noted that these projections assume that beryllium is present in the coal and sorbent feed in a matrix-free form. If beryllium is instead present in some complex form, the fate of beryllium in the fluid-bed combustion systems could be different from that projected here. One aspect of this possibility is discussed below.

Consideration must be given to the reaction of beryllium with aluminum and silicon, the major clay constituents of coal. Calculations indicate that in the presence of excess aluminum, the stable form of solid $BeO \cdot 3\ Al_2O_3$ is produced. Introduction of magnesium and silicon to the system alters the reaction in such a manner that aluminum does not stoichiometrically re-form in the 6:1 ratio (forming $BeO \cdot 3\ Al_2O_3$), but forms the stable $BeO \cdot Al_2O_3(s)$ in addition to magnesium aluminate, $MgO \cdot Al_2O_3(s)$; magnesium silicate, $MgO \cdot SiO_2(s)$; silicon dioxide, $SiO_2(s)$; aluminum silicate, $Al_2O_3 \cdot SiO_2(s)$; and aluminum hydroxide, $Al(OH)_3(s)$. Figure 8 illustrates the reactions of beryllium, as a trace element, with the clay constituents of coal.

In order to illustrate the effect aluminum has on the production of gaseous beryllium hydroxide, profile plots of the $BeO \cdot Al_2O_3/Be(OH)_2$

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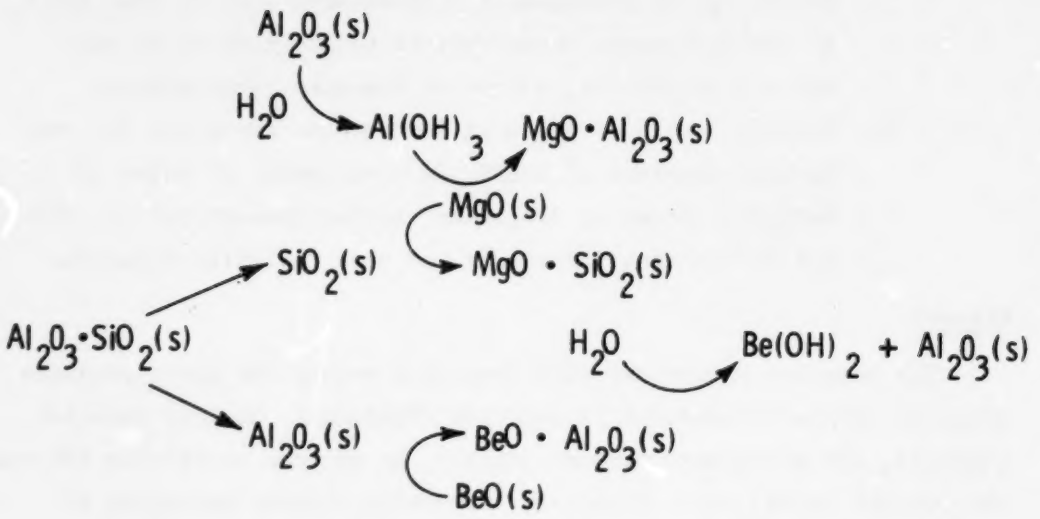

Figure 8. Chemical Equilibrium Reactions of Beryllium with Clay Constituents of Coal.

system are presented in Figures 9 and 10 for comparison with those of the $BeSO_4/Be(OH)_2$ equilibrium system (Figures 11 and 12). The following have been noted:

- In the $BeO \cdot Al_2O_3/Be(OH)_2$ system
  1. $BeSO_4(s)$ is not stable, even at low temperatures
  2. $Be(OH)_2(g)$ is produced as the major beryllium compound at temperatures greater than 400 K, indicative of $BeO \cdot Al_2O_3(s)$ removal.
- In the $BeSO_4/Be(OH)_2$ system
  1. $Be(OH)_2(g)$ is produced at temperatures greater than 600 K at concentrations comparable to those produced in the $BeO \cdot Al_2O_3/Be(OH)_2$ system at elevated temperatures.
  2. Tables 5 and 6 of Appendix A should be consulted for the partial pressure of $Be(OH)_2(g)$ and number of moles of $BeSO_4(s)$ formed at 90 percent sulfur removal for 10, 100 and 300 percent excess air for high coal-high dolomite.

Mercury

The reaction of mercury with fluid-bed combustion gases produces volatile species of mercury II chloride ($HgCl_2(g)$), mercury monoxide (HgO(g)), and monoatomic mercury (Hg(g)), in systems containing 100 and 300 percent excess air. Fluid-bed combustion systems operating at 10 percent excess air additionally form diatomic mercury (Hg_2), mercury chloride (HgCl), mercurous chloride (Hg_2Cl_2), and mercury monohydride (HgH).

Mercury II chloride is the favored trace chlorine compound that forms at low temperatures. Mercury II chloride gas is stable below 900 K; above this temperature HCl is released from the complex with the production of gaseous mercury and further oxidation of mercury to HgO:

$$HgCl_2(g) \longrightarrow Hg(g) + Cl_2(g) \qquad (14)$$

$$Hg(g) + 1/2\ O_2(g) \longrightarrow HgO(g)\ . \qquad (15)$$

System: C-H-N-O-S-Cl-K-Mg-Al-Si-Be

BE(OH)2 Gas: Partial Pressure

temp (K)	1.0 atm	5.0 atm	10.0 atm
300.0	3.5390-12	1.6030-10	2.4270-09
400.0	5.6410-07	3.7730-07	3.1720-07
500.0	5.7660-07	2.8930-06	5.7870-06
600.0	5.7840-07	2.8920-06	5.7840-06
700.0	5.7840-07	2.8920-06	5.7840-06
800.0	5.7840-07	2.8920-06	5.7840-06
900.0	5.7840-07	2.8920-06	5.7840-06
1000.0	5.7910-07	2.8960-06	5.7910-06
1100.0	5.7830-07	2.8940-06	5.7870-06

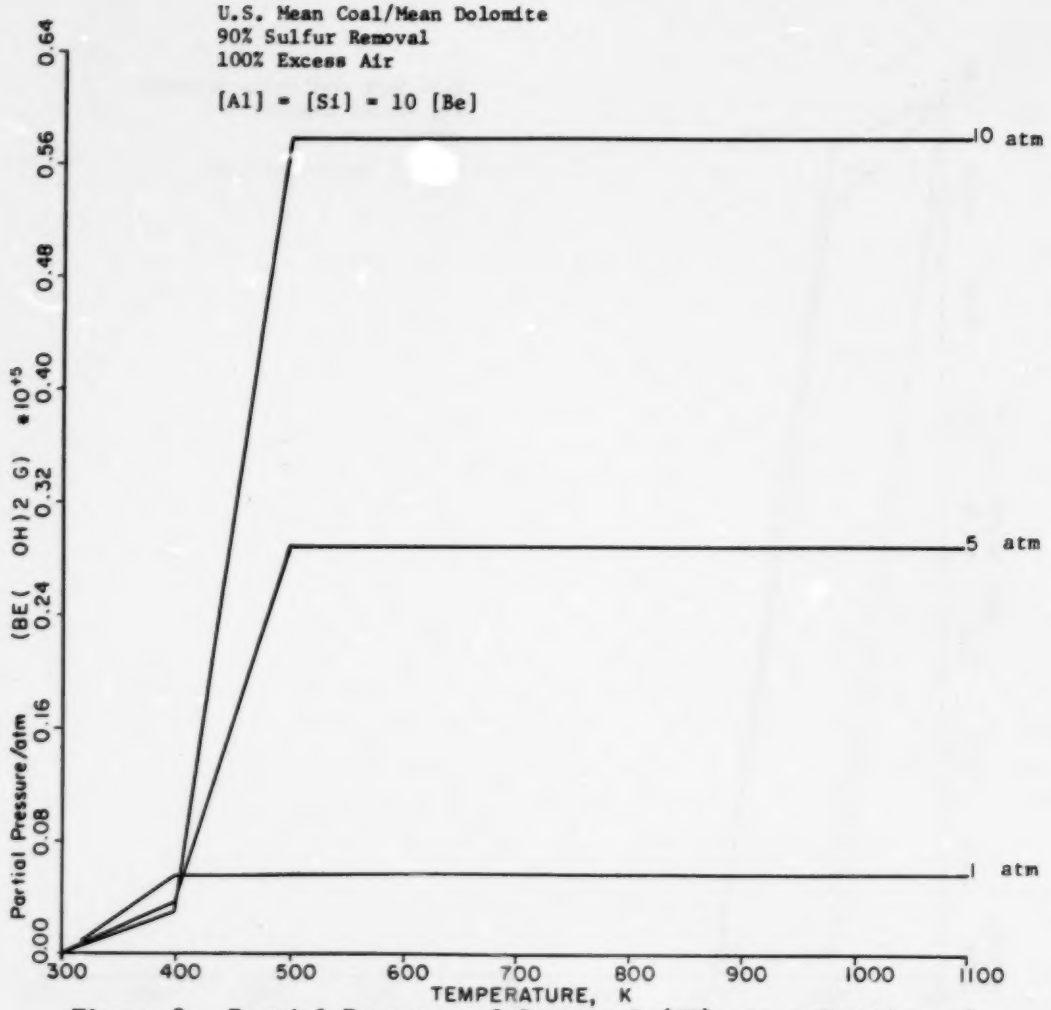

Figure 9. Partial Pressure of Gaseous $Be(OH)_2$ as a Function of Temperature and Pressure. Interaction between Beryllium and Aluminum Produces a Solid Complex of $BeO \cdot Al_2O_3$ at Low Temperatures. Production of Gaseous $Be(OH)_2$ Is Dependent on the Volatilization of Be from This Complex.

System: C-H-N-O-S-Cl-K-Mg-Al-Si-Be

temp (K)	1.0 atm	5.0 atm	10.0 atm
300.0	3.9210-05	3.9160-05	3.9180-05
400.0	1.0220-06	3.4120-05	3.7080-05
500.0	.0000	.0000	.0000
600.0	.0000	.0000	.0000
700.0	.0000	.0000	.0000
800.0	.0000	.0000	.0000
900.0	.0000	.0000	.0000
1000.0	.0000	.0000	.0000
1100.0	.0000	.0000	.0000

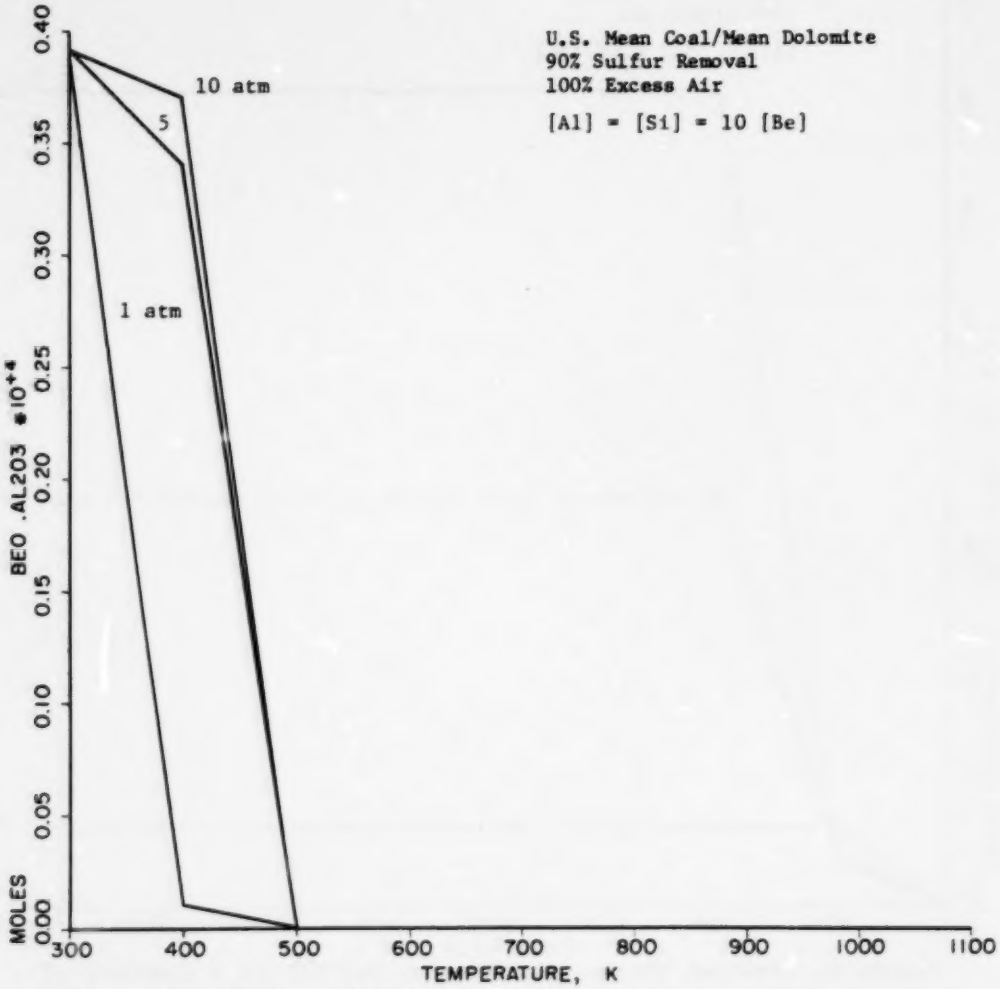

Figure 10. Number of Moles of Solid $BeO \cdot Al_2O_3$ as a Function of Temperature and Pressure Produced When Aluminum Is Presented at Ten Times the Beryllium Level for U. S. Mean Coal Systems.

System: C-H-N-O-S-Cl-K-Be

BE(OH)2 Gas: Partial Pressure

temp (K)	1.0 atm	5.0 atm	10.0 atm	15.0 atm
300.0	3.9390-23	1.3170-22	2.2150-22	3.0020-22
400.0	8.4290-16	2.8190-15	4.7400-15	6.4250-15
500.0	2.1990-11	7.0290-11	1.1760-10	1.5900-10
600.0	5.7540-07	2.8790-06	5.7590-06	1.6480-07
700.0	5.7540-07	2.8790-06	5.7580-06	1.6480-07
800.0	5.7570-07	2.8790-06	5.7570-06	8.6360-06
900.0	5.7560-07	2.8780-06	5.7650-06	8.6350-06
1000.0	5.7660-07	2.8700-06	5.7560-06	8.6340-06
1100.0	5.7650-07	2.8690-06	5.7570-06	8.6450-06

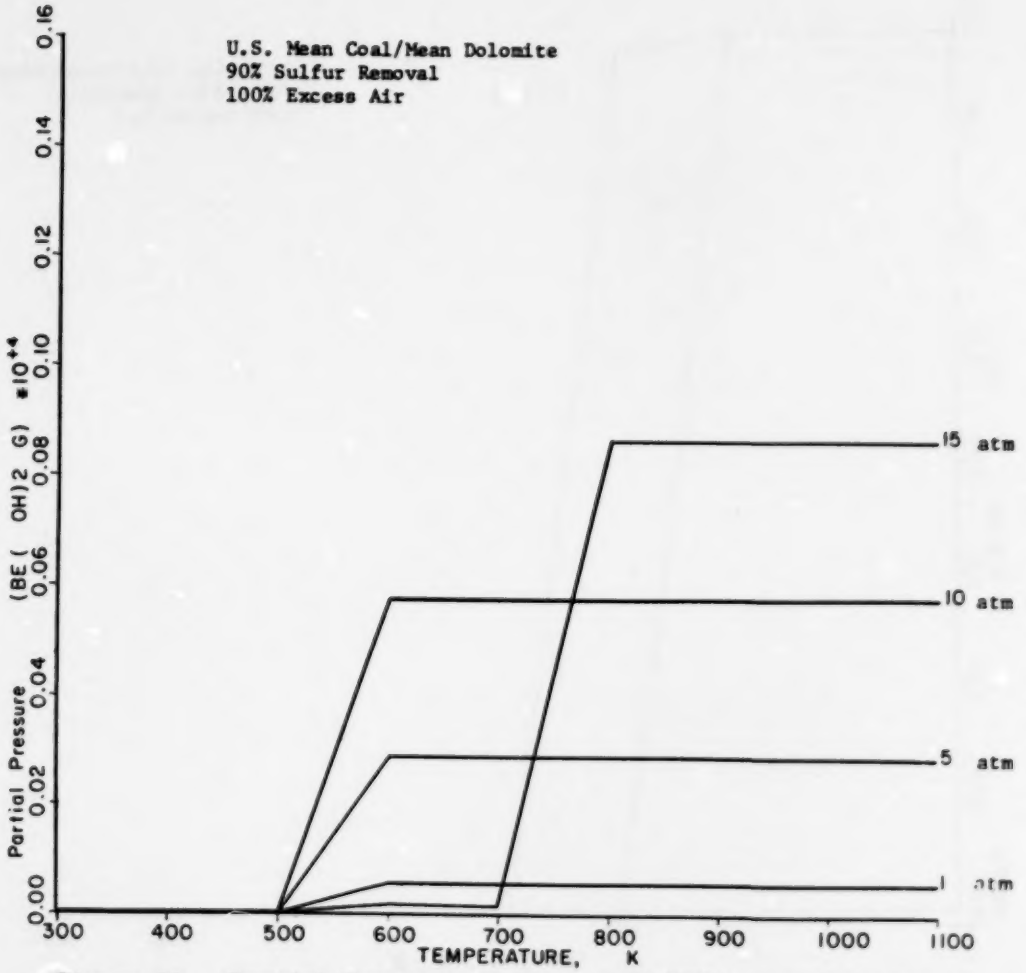

Figure 11. Partial Pressure of Gaseous $Be(OH)_2$ as a Function of Temperature and Pressure without Be/Al-Si Interaction. Production of Gaseous $Be(OH)_2$ Is Dependent on the Volatilization of Solid $BeSO_4$.

System: C-H-N-O-S-Cl-K-Be

temp (K)	1.0 amp	5.0 atm	10.0 atm	15.0 atm
300.0	3.9180-05	3.9180-05	3.9180-05	3.9180-05
400.0	3.9180-05	3.9180-05	3.9180-05	3.9180-05
500.0	3.9190-05	3.9190-05	3.9180-05	3.9180-05
600.0	.0000	.0000	.0000	3.8340-05
700.0	.0000	.0000	.0000	.0000
800.0	.0000	.0000	.0000	.0000
900.0	.0000	.0000	.0000	.0000
1000.0	.0000	.0000	.0000	.0000
1100.0	.0000	.0000	.0000	.0000

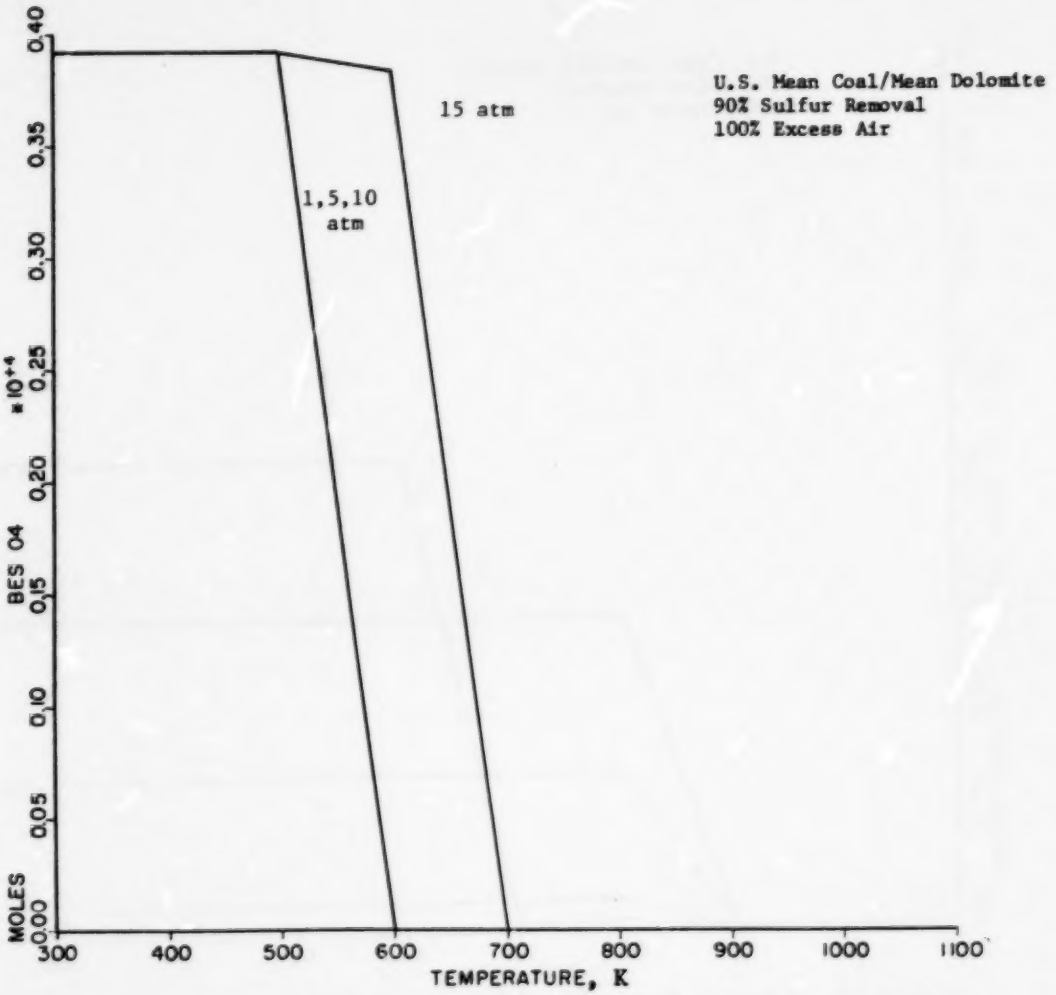

Figure 12. Number of Moles of Solid $BeSO_4$ as a Function of Temperature and Pressure without Be/Al-Si Interaction.

At reduced pressures and elevated temperatures removal of $HgCl_2$ from the gas phase is enhanced. Similarly, reduction of the sulfur concentration in fluid-bed gases further reduces the partial pressure of the $HgCl_2$ due to the increased oxygen partial pressure in the system, favoring reaction 15. This is illustrated by comparison of the partial pressure of $HgCl_2$ at 1200 K:

	SYSTEM TOTAL PRESSURE	
Sulfur Removal, %	15 atm	1 atm
0	3.753×10^{-10} atm	2.053×10^{-13} atm
99	1.119×10^{-13} atm	8.191×10^{-17} atm

The trace level of mercury used in the equilibrium calculations for all fluid-bed combustion systems is on the order of 10^{-7} moles (see Table 4). Relative concentrations of this magnitude are sufficiently low to produce a 1-to-4 percent mass constraint error. This error is significant for the trace level of mercury, so caution must therefore be exercised when comparing results quantitatively for the mercury compounds.

Trace levels ($<10^{-12}$ atm) of $Hg_2(g)$ and HgCl(g) are projected to form in fluid-bed gases. Reduction in the concentration of sulfur to 99 percent removal produces a greater partial pressure of Hg_2 and of HgCl at low temperatures than in the 0-to-90 percent sulfur removal systems. Equivalence in the partial pressure exerted by $Hg_2(g)$ for the 0-to-90 and 99 percent removal systems, is reached at elevated temperatures. Gaseous HgCl is not detected in systems containing 300 percent excess air.

Tables 7 through 11 of Appendix A illustrate the partial pressures for the gaseous mercury compounds formed in fluid-bed combustor gases. The results are determined for the high coal-high dolomite system with 90 percent sulfur removal. Solids and sulfate compounds of mercury

are not projected to form stable phases under any fluid-bed condition. Mercury released as a gas should not condense in the cooling stages of the process. Complete volatilization of mercury in the coal or sorbent is projected with emission from the stack in the form of oxides and chlorides that are capable of entrainment on the surface of particulates in the gas stream.

Lead

The volatile compounds lead tetrachloride, $PbCl_4$; lead dichloride, $PbCl_2$; lead chloride, PbCl; and lead oxide, PbO, are projected to be formed when lead is present in fluid-bed combustion gases. Over the temperature range of 300 to 1200 K, lead tetrachloride is the predominant gaseous trace compound. Formation of $PbCl_4$ results from the reaction of PbO with HCl as shown by the reaction:

$$PbO(g) + 4\ HCl(g) + 1/2\ O_2 \longrightarrow PbCl_4(g) + 2\ H_2O(g)\ . \qquad (16)$$

Reducing the sulfur level (i.e., 99 percent sulfur removal) increases the partial oxygen pressure and limits the formation of gaseous $PbCl_4$ at low pressures when the temperature is greater than 1000 K (reverse of reaction 16). Bet een 1000 and 1100 K, $PbCl_4$ releases chlorine, reducing the concentration of the $PbCl_4$ while increasing the $PbCl_2$ (reaction 17):

$$PbCl_4(g) \longrightarrow PbCl_2(g) + 2\ Cl(g)\ . \qquad (17)$$

Reduction of the pressures at elevated temperatures causes a further transition of the $PbCl_2$ phase. Chlorine is removed from $PbCl_2$, forming gaseous PbCl:

$$PbCl_2(g) \longrightarrow PbCl(g) + Cl(g)\ . \qquad (18)$$

Reducing the sulfur level from 90 to 99 percent produces a dramatic increase in the partial pressure of PbO. Only a light change is

detected, however, between the 0 to 90 percent systems. At 1200 K and 15 atmospheres the partial pressures of PbO for the 10 and 100 percent excess air cases are as follows:

	Excess Air	
Sulfur Removal, %	10%	100%
0	1.273×10^{-9} atm	1.056×10^{-9} atm
90	1.376×10^{-9} atm	1.265×10^{-9} atm
99	1.559×10^{-5} atm	8.899×10^{-6} atm

Tables 12 through 15 of Appendix A illustrate the partial pressures for volatile lead compounds produced by fluid-bed combustion systems with 90 percent sulfur removal.

Fluorine, Beryllium, Mercury, Lead System

The equilibrium reactions of fluid-bed combustion gases do not project the interaction of trace elements. For example, fluorine and mercury do not form stable phases of mercurous fluoride, FHg and F_2Hg_2, or mercuric fluoride, F_2Hg, as either solids, liquids, or gases. Similarly, fluorine does not react with lead-forming trace complexes of lead mono-, di-, or tetrafluorides, (FPb, F_2Pb, or F_4Pb). Oxy-fluorides and fluorides do not combine with beryllium, nor do chlorides of beryllium-fluorine result (i.e., BeClF).

PARAMETRIC FBC EQUILIBRIUM CONCENTRATIONS

The reactions of the trace elements in fluid-bed combustors act as individual systems, producing the chlorides, sulfates, and oxides of the particular element. Tables 8, 9, and 10 summarize the distribution of the trace elements in various gaseous and solid phases for 90 percent sulfur removal conditions in 10, 100, and 300 percent excess air for high coal-high dolomite systems. It is evident that temperature influences the form in which the trace element is most stable, as well as the variations in the distribution of the element with total system pressure.

TABLE 8. DISTRIBUTION OF TRACE ELEMENTS IN HIGH COAL-HIGH DOLOMITE SYSTEMS FOR 10% EXCESS AIR - 90% SULFUR REMOVAL

FRACTIONAL DISTRIBUTION OF THE TRACE ELEMENTS AMONG THEIR PRINCIPAL COMPOUNDS - (GASEOUS UNLESS OTHERWISE NOTED)

Trace Compound	1200 K		300 K	
	15 atm	1 atm	15 atm	1 atm
HF	0.99	0.99	1.70×10^{-3}	1.70×10^{-3}
KF	4.64×10^{-5}	1.11×10^{-3}	--	--
NaF	1.38×10^{-5}	3.29×10^{-4}	--	--
SO_2F_2	2.79×10^{-7}	7.30×10^{-9}	0.99	0.99
$BeSO_4$(s)	--	--	0.99	0.99
$Be(OH)_2$	1.00	1.00	3.95×10^{-16}	7.71×10^{-16}
Hg	0.96	0.99	9.34×10^{-29}	1.41×10^{-27}
HgO	3.70×10^{-2}	9.90×10^{-3}	1.39×10^{-27}	5.40×10^{-27}
$HgCl_2$	4.53×10^{-3}	1.93×10^{-5}	0.97	0.97
$PbCl_4$	0.99	0.31	0.99	0.99
$PbCl_2$	3.31×10^{-3}	0.25	--	--
PbCl	1.21×10^{-5}	1.44×10^{-2}	--	--
PbO	8.71×10^{-5}	0.42	--	--
NaCl	2.93×10^{-2}	0.34	--	--
NaOH	8.83×10^{-5}	2.11×10^{-3}	--	--
Na_2SO_4	8.33×10^{-5}	1.25×10^{-3}	--	--
Na_2SO_4(s)	0.97	0.65	1.00	1.00
KCl	3.63×10^{-2}	0.42	4.16×10^{-35}	3.16×10^{-34}
KOH	2.14×10^{-5}	5.11×10^{-4}	--	--
K_2SO_4	2.73×10^{-3}	4.09×10^{-2}	--	--
K_2SO_4(s)	0.96	0.54	1.00	1.00

SYSTEM: C-H-N-O-S-Cl-K-Na-F-Be-Hg-Pb.

TABLE 9. DISTRIBUTION OF TRACE ELEMENTS IN HIGH COAL-HIGH DOLOMITE SYSTEMS FOR 100% EXCESS AIR - 90% SULFUR REMOVAL

FRACTIONAL DISTRIBUTION OF THE TRACE ELEMENTS AMONG THEIR PRINCIPAL COMPOUNDS - (GASEOUS UNLESS OTHERWISE NOTED)

Trace Compound	1200 K		300 K	
	15 atm	1 atm	15 atm	1 atm
HF	0.99	0.99	1.70×10^{-3}	1.70×10^{-3}
KF	6.11×10^{-5}	1.38×10^{-3}	—	—
NaF	1.82×10^{-5}	4.09×10^{-4}	—	—
SO_2F_2	2.86×10^{-7}	8.37×10^{-9}	0.99	0.99
$BeSO_4$(s)	--	—	0.99	0.99
$Be(OH)_2$	1.00	1.00	7.57×10^{-16}	1.49×10^{-15}
Hg	0.98	0.93	1.36×10^{-28}	2.56×10^{-27}
HgO	7.79×10^{-2}	1.92×10^{-2}	4.17×10^{-27}	2.03×10^{-26}
$HgCl_2$	5.20×10^{-3}	1.65×10^{-5}	0.79	0.99
$PbCl_4$	0.99	0.19	1.00	1.00
$PbCl_2$	3.00×10^{-3}	0.17	—	—
PbCl	1.01×10^{-5}	1.01×10^{-2}	—	—
PbO	1.42×10^{-4}	0.63	—	—
NaCl	3.80×10^{-2}	0.38	—	—
NaOH	1.16×10^{-4}	2.63×10^{-3}	—	—
Na_2SO_4	1.48×10^{-4}	2.22×10^{-3}	—	—
Na_2SO_4(s)	0.96	0.62	1.00	1.00
KCl	4.70×10^{-2}	0.47	—	2.94×10^{-34}
KOH	2.82×10^{-5}	6.36×10^{-4}	—	—
K_2SO_4	4.85×10^{-3}	7.27×10^{-2}	—	—
K_2SO_4(s)	0.95	0.46	1.00	1.0

SYSTEM: C-H-N-O-S-Cl-K-Na-F-Be-Hg-Pb.

TABLE 10. DISTRIBUTION OF TRACE ELEMENTS IN HIGH COAL-HIGH DOLOMITE SYSTEMS FOR 300% EXCESS AIR - 90% SULFUR REMOVAL

FRACTIONAL DISTRIBUTION OF THE TRACE ELEMENTS AMONG THEIR PRINCIPAL COMPOUNDS - (GASEOUS UNLESS OTHERWISE NOTED)

Trace Compound	1200 K		300 K	
	15 atm	1 atm	15 atm	1 atm
HF	0.99	0.99	1.70×10^{-3}	1.70×10^{-3}
KF	1.10×10^{-4}	2.40×10^{-3}	--	--
NaF	3.28×10^{-5}	7.11×10^{-4}	--	--
SO_2F_2	1.73×10^{-7}	5.42×10^{-9}	0.99	0.99
$BeSO_4(s)$	--	--	0.99	0.99
$Be(OH)_2$	0.99	0.99	1.17×10^{-15}	2.31×10^{-15}
Hg	0.97	0.93	3.76×10^{-28}	5.16×10^{-27}
HgO	9.40×10^{-2}	2.34×10^{-2}	1.41×10^{-26}	5.00×10^{-26}
$HgCl_2$	2.89×10^{-3}	4.96×10^{-6}	1.11	1.02
$PbCl_4$	0.99	2.02×10^{-2}	0.99	0.99
$PbCl_2$	5.25×10^{-3}	6.00×10^{-2}	—	—
PbCl	2.41×10^{-5}	6.53×10^{-3}	—	—
PbO	5.51×10^{-4}	0.91	—	—
NaCl	6.53×10^{-2}	0.48	—	—
NaOH	2.10×10^{-4}	4.58×10^{-3}	—	—
Na_2SO_4	2.92×10^{-4}	4.38×10^{-3}	—	—
$Na_2SO_4(s)$	0.93	0.53	1.00	1.00
KCl	8.09×10^{-2}	0.57	—	—
KOH	5.08×10^{-5}	1.11×10^{-3}	—	—
K_2SO_4	9.55×10^{-3}	0.14	—	—
$K_2SO_4(s)$	0.91	0.29	1.00	1.00

SYSTEM: C-H-N-O-S-Cl-K-Na-F-Be-Hg-Pb.

In order to demonstrate that the trace compounds formed in high coal-high dolomite systems are produced in fluid-bed combustion systems that use various grades of coals and sulfur sorbents, the equilibrium composition was calculated for mean coal-mean dolomite conditions and mean coal-low dolomite conditions. Parametrically, these conditions define the upper, middle, and lower limits of the trace element concentrations. In varying the level of each constituent, no change in chemical form is observed in the final trace products. The active compounds for mean coal-low dolomite are identical with those that result in high coal-high dolomite systems. The only change that should be noted when using an alternative system is that the level of the gaseous trace compound reflects the initial trace concentration in the coal and sorbent feedstock. Tables 1 through 4 of Appendix B indicate the partial pressures of the gaseous trace compounds produced at 1200 K for operating conditions of 100 percent excess air, with 90 percent sulfur removal for high coal-high dolomite and mean coal-low dolomite systems. Note the difference in the partial pressures of each compound when the initial levels of the trace constituents are varied (see Table 4 of Section 4 for initial concentrations).

The partial pressures of the trace compounds that result in high coal-high dolomite systems have been calculated as a function of the excess air content. For all sulfur removal systems operating between 1 and 15 atmospheres at temperatures of 1200 K, the partial pressures of the trace compounds HF, KF, NaF, $Be(OH)_2$, $HgCl_2$, HgCl, HgO, $PbCl_4$, and $PbCl_2$ are shown to be suppressed as more air is supplied to the combustion process. This is simply a dilution effect. The partial pressures of PbO and PbCl are projected to slightly increase in 300 percent excess air for 0-to-90 percent sulfur removal conditions at high system pressures.

The thermochemical properties of the trace fluid-bed combustion system were calculated (as part of the computer program subroutine) (Appendix C). Variations between trace systems as compared with pure

fluid-bed gases exist only within the sixth decimal position. The properties for systems with and without trace elements are virtually the same.

ASSESSMENT

The thermodynamic analysis performed shows that essentially all of the beryllium, lead, mercury, and fluorine can be volatilized at the normal operating temperatures, pressures, and sulfur dioxide levels in fluidized-bed combustion. These projections assume that all of these trace metals are present in the coal and sorbent feedstocks in a matrix-free form, available for the reactions considered. For beryllium and fluorine species, some condensation will occur on cooling the gases through reactions of the trace element phases with the carbonate and clay fractions of the coal and sorbent. The gaseous species of lead and mercury when formed do not condense at ambient temperatures. No significant interaction between these trace elements is projected, and no significant differences between pressurized and atmospheric-pressure operation were noted, except for lead, as discussed below.

These projections may be compared with the mass balances performed by Argonne National Laboratories (ANL)[7] around a pressurized fluidized-bed combustion system. In their experiments, ANL found that of the four elements mentioned above, good retention (≈100 percent) of lead was noted in the solids phase, but the average retention of the other elements was only 42 percent, despite the relatively low temperature (600-800°F) at which overhead samples were collected. This power retention in the solid phases is in agreement with the projections reported in this study, although this study reports even poorer retention than that which Argonne observed. It is significant to note that the retention of fluorine in the ANL experiments was much higher (56-62 percent) with a calcium sorbent than with a sorbent-free bed (5-23 percent), agreeing further with the projections made in this

study. The projections shown here indicate that cooling the gas with excess CaO, as normally present in fines, leads to retrapment of the liberated fluorine.

It is surprising that lead retention is predicted thermodynamically to be poor in pressurized systems.[1] In the Argonne experiments both lead and beryllium were concentrated in the finer particles (indicating redeposition on cooling). In measurements to determine the fate of elements in a cyclone-fed power plant, Fulkerson et al. (Oak Ridge)[24] found that 10 percent of the lead was lost as an atmospheric discharge. This makes the predicted volatilization of lead as $PbCl_4$ unlikely, and several reasons can be advanced. The kinetics of conversion of the other lead compounds to $PbCl_4$ may be intrinsically slow, or the lead may be bound up in the mineral matter in a form that is not very accessible to the HCl content of the gas. Alternatively, there may be more stable compounds of lead - silicates or borates - than those considered here. In addition, conversion of lead to $PbCl_4$ is initially dependent on the concentration of HCl in the gas. If the HCl level falls to 50 percent of its assumed value, then $PbCl_4$ falls to 6 percent of its previous value. This can be seen by examining the mean coal-low dolomite case in Table 4 of Appendix B, where for the atmospheric pressure case, PbO(g) is the predominant lead compound. In this case, lead will quickly condense on particulate matter on cooling. The circumstances that favor PbO are, therefore, low-pressure operation and low HCl release, which would occur with a low-chlorine coal or when alkali release is high enough to lower the free HCl content of the gas.

EXTENSION OF THERMODYNAMIC PROJECTIONS TO OTHER ELEMENTS PRESENT IN COAL, USING ELEMENT VOLATILITY AS A CRITERION

Consideration was given to choosing a representative selection of additional elements based upon the classification of trace elements and upon the concentration of the element in coal. (Refer to

Table 11.) The selection of four trace elements (bromine, molybdenum, antimony, and vanadium) resulted from reported volatile loss in high- and low-temperature ashing processes. Thermodynamic data available for these four elements were reviewed from the work of JANAF and Barin and Knache:

- Br - data for complexes forming Cl-H-N-O-K-Na-Pb-Hg-Mg, etc.
- Mo - data for Cl-O-F-H readily available
- Sb - not reported in JANAF
- V - oxides and nitrides - limited.

On the basis of available data bromine and molybdenum are good choices; and antimony and vanadium would take an additional literature review and estimates to fit reported data. Substitution may be made, with phosphorus and boron both showing reasonable data in JANAF, and both can be used to demonstrate interaction with the previous Be-F-Hg-Pb study. Toxicity data, which is included in Table 11, should not be used as a major deciding factor since the levels are listed for compounds found in NIOSH and may not include pertinent species that form in the fluid-bed system.

TABLE 11. TRACE ELEMENTS IN COAL

Trace Element	Classification	Comment	TWA[a]	Concentration	Data Bank
As	Mineral matter				
B	Organic affinity Clean coal		B_2O_3 = 15 mg/m^3	102 ppm	Boron complexes with Br, O, Cl, F, H, Li, K, Be, F, Pb, K, Mg
Be	--	Completed	--	--	--
Br		Volatiles lost in LTA[b] ∿100%	Br_2 = 0.1 ppm	15.42 ppm	Bromium complexes Cl, F, H, N, Hg, K, Mg, N, Na, P, Pb
Cd	Mineral matter				
Co	Combination				
Cr	Combination				
Cu	Combination				
F	--	Completed	--	--	--
Ga	Organic and inorganic affinity				
Ge	Organic affinity clean coal				
Hg	--	Completed	--	--	--
Mn	Mineral matter				
Mo	Mineral matter	Lost in HTA[c] ∿33%	MnO_3 = 7.5 mg/m^3	7.54 ppm	Oxide complexes
Ni	Combination				
P	Organic and inorganic affinity		$PbCl_3$ = 0.5 ppm P_2S_5 = 1 mg/m^3	71.1 ppm	Oxide, chloride and sulfide complexes
Pb	--	Completed	--	--	--
Sb	Organic and inorganic	Volatiles lost in LTA ∿5%		1.26 ppm	Not reported
Se	Combination				
U	Inorganic				
V	Organic and inorganic	Lost in HTA ∿25%	V_2O_5 = 1 mg/m^3 /8hrs (TCLo)[d]	32.71 ppm	Oxides nitrides
Zn	Mineral matter				
Zr	Mineral matter				

[a] TWA - Time Weighted Average
[b] LTA - Low-Temperature Ashing
[c] HTA - High-Temperature Ashing
[d] TCLo - Lowest Published Toxic Concentration

SECTION 6

EXPERIMENTAL DETERMINATION

APPROACH

The thermodynamic projections reported indicate potential pathways for the release of trace elements into the gaseous effluent from the fluidized-bed combustion system. On the other hand, a limited number of experimental studies have been carried out to analyze the effluent streams and characterize their actual trace element content. These studies are of immense value, but they do not cover the ranges of proposed operating conditions or possible design applications. Since our major objective is to attempt to characterize and evaluate emissions before development of full-scale systems, an intermediate experimental study is required, in which the kinetics of trace element release are studied over a range of simulated fluidized-bed combustor operating conditions.

Previous experimental studies at Westinghouse on the release of trace elements from fluidized-bed combustion feedstock materials have concentrated on the principal elements that induce corrosion on boiler tubes and turbine metal surfaces - namely, sodium and potassium. A custom-built flame-emission spectroscopic apparatus was used to monitor continuously the release of these elements from coal ash and dolomite sorbents and to study the use of getter materials to suppress alkali release. Because this apparatus can be used to simulate the effect of a number of important operating variables - temperature, gas composition, particle size, coal type, and sorbent type - it was thought worthwhile to assess its use in an extended program to measure the kinetics of release of potentially volatile trace metals such as lead

and mercury under fluidized-bed combustor operating conditions. The experimental program was limited to ascertaining the utility of the existing apparatus for this purpose, and only minor modifications were considered.

FLAME EMISSION SPECTROPHOTOMETRY

The flame emission spectroscopic technique, used for the continuous monitoring of sodium- and potassium-bearing vapors that are released from heated samples of dolomite stones, is shown by the schematic drawing of Figure 13. A known quantity of sample matter is filled into a nickel boat and placed inside a nickel tube that serves as a heating susceptor for the RF radiation. The sample temperature is monitored with an Inconel-sheathed thermocouple, the hot junction of which is near the sample bucket. A controlled flow of a synthetic gas mixture is passed through the tubular nickel crucible. Volatile material given off the sample is carried with the gas without appreciable cooling through a reduced opening into a hydrogen/oxygen flame. Hydrogen and oxygen are piped through annular tubes to the burner nozzle. A laminar flow of nitrogen keeps the outer quartz tubing free from deposits and protects it from overheating in the area around the flame.

A uniform section of the diffusion flame is focused on the inlet slit of a Jarrel-Ash spectrometer. A portion of the spectrum is picked up by an image intensifier tube. The signals are digitized and displayed on a TV tube. Hollow cathode light sources are used to preset the optical and recording system and maximize the signal output. The maximum characteristic line intensity (5896 Å for sodium and 7665 Å for potassium) is plotted out on a strip chart recorder, although digital data handling and reduction would be preferable.

In order to quantify the emission signal from sodium and potassium radiation, known amounts of NaCl and KCl are completely vaporized into the gas stream. The signal-time integral of the known standard is applied as a unit measure to quantify the accumulated signal of an unknown sample.

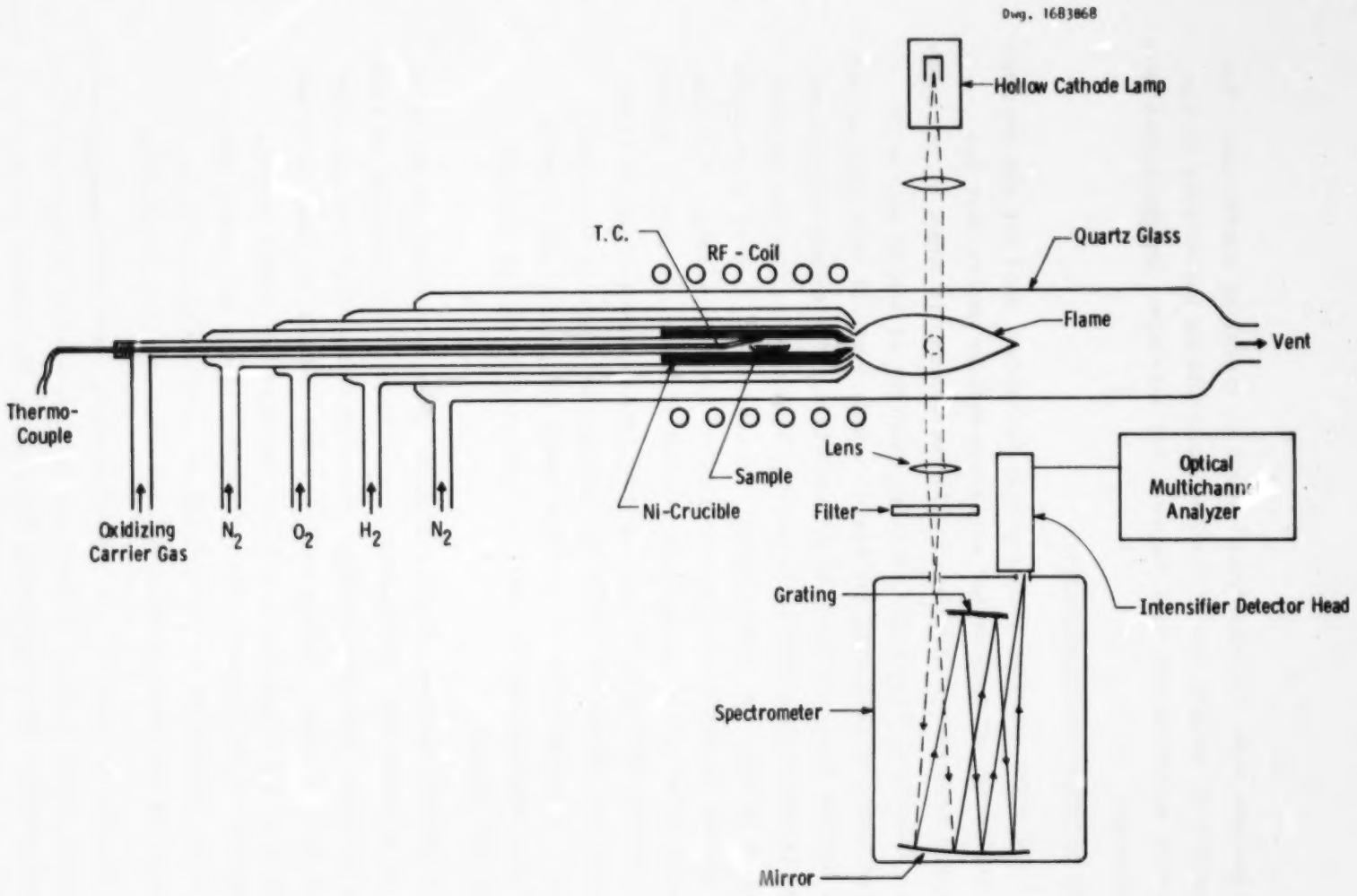

Figure 13. Apparatus for the Flame Spectroscopic Determination of Alkali Release from Feed Materials in the Fluidized-Bed Combustors.

A typical emission intensity-versus-time output curve plotted on a strip chart recorder is shown in Figure 14. The shaded area covers the width of intensity fluctuations that may be caused by local variations of the release of alkali vapors. The magnitude of the recorded signal and the shape of the curve depend on the temperature, the geological origin of the dolomite, and the total alkali impurity content. Generally, the characteristic alkali signal reaches a maximum quickly, as soon as the desired final temperature is attained. The signal drops off, at first abruptly, and then more gradually, falling to a very low quasi-steady value. The intensity charts were graphically integrated and quantified by comparison with intensity curves from known KCl or NaCl standards. The results of the calculation are alkali release curves that give the accumulated amount of released alkali in μg as a function of time, as shown in Figure 15.

In order to obtain reproducible results, parameters such as the hydrogen, oxygen, and synthetic combusted gas flow rates must be accurately controlled. The shape of the combustor nozzle and the effusion hole of the susceptor can appreciably affect the emission signal. Calibration runs have to be periodically repeated, particularly after replacing the combustor or nickel susceptor, in order to take small uncontrollable changes of the calibration factor into account. Care must also be taken that the alkali vapor density in the flame does not exceed an upper level, above which linearity between emission signal and concentration is impaired. If the emission signal becomes too high, the sample size has to be appropriately reduced.

Apparatus Modifications

Any changes required to test the signal output of the flame emission spectrum of the toxic elements (lead, mercury, etc.) were made in the spectroscopic and detector components of the apparatus. In order to gain an insight into the difficulties that may be encountered in using this technique for the continuous monitoring of the toxic trace

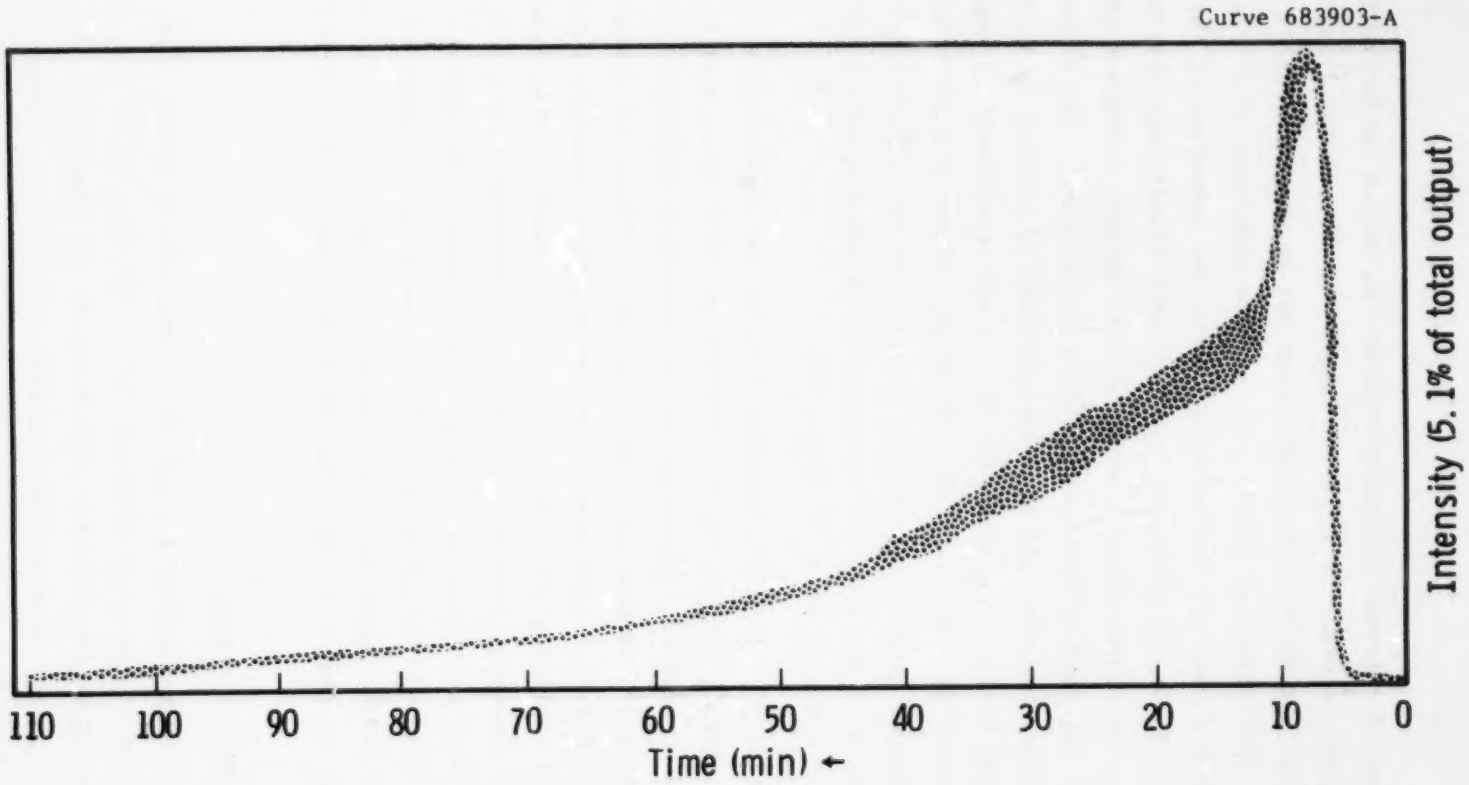

Figure 14. Flame Emission Intensity-Time Curve Illustrating the Release of Potassium Vapor Impurity from 300 mg of Tymochtee Dolomite at 875°C in Flowing Fuel Gas (22.1% H_2/19.4% CO/18.2% CO_2/40.3% N_2 at 75 cc/min)

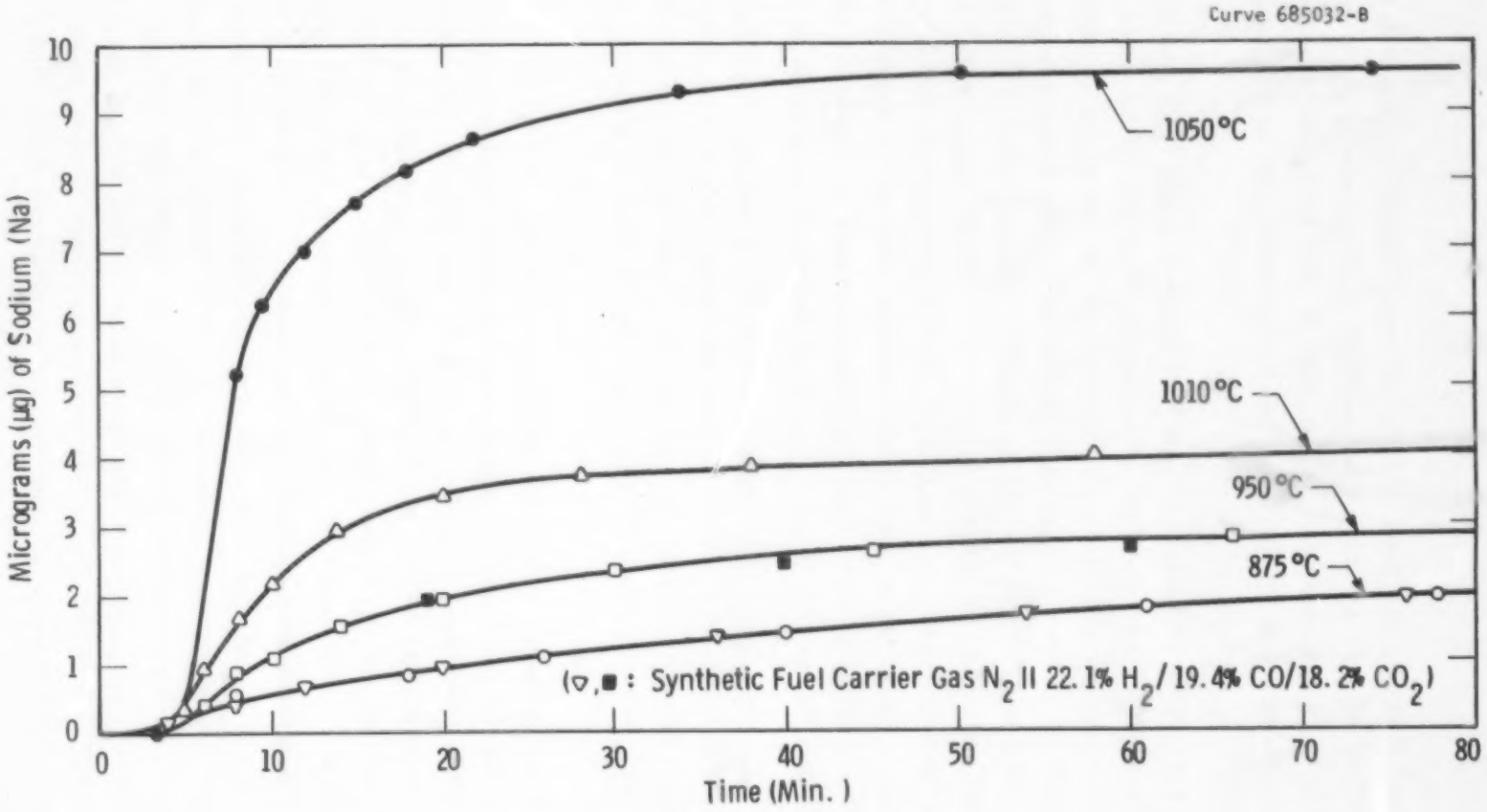

Figure 15. Release of Na from Geneva Dolomite. (Sample Weight 100 mg; Particle Size, 35-40 Mesh - ASTM; Carrier Gas: 19.8% CO_2/2.2% O_2//N_2 at 75 cc/min.; Na Concentration in Sample: 204 ± 13 ppm)

element release, the total content of these traces in the coal feed materials as well as their spectrochemical properties must be considered. In the case of coal ash samples that have been prepared at temperatures below 700°C, the total lead content can be as high as 50 ppm.[25]

For 100 mg of such a sample (the maximum capacity of the nickel sample holder), the absolute total amount of lead will be about 5 µg. Only 1 to 10 percent (i.e., 0.05 to 0.5 µg) of this lead is expected to be released at coal combustion temperatures. The strong resonance line for lead (4059 Å) yields an emission signal a factor of ∿100 less intense than that of the K-line (7665 Å). Taking these latter two facts in conjunction, the magnitude of the difficulties becomes rather obvious. Furthermore, even if the optimum position of the permissible hydrogen/oxygen flame in this apparatus is employed, the spectral response may be even less than the above quoted factor of 100.

Mercury probably will be more difficult to monitor than lead, since mercury is expected to be less sensitive than lead in the flame emission mode by a factor of ∿20, and its total content in the same materials is expected to be less than that of lead by a factor of ∿100.[25]

A Westinghouse commercial hollow cathode lamp was always used to preset the emission signal output. The entrance straight slit to the Jarrel Ash spectrometer (Model No. 82-000) was 100 µm. The optimum flame emission volume was found to be close to the beginning of the outer zone of the diffusion flame. In the case of lead, in addition to the previously used Silicon Intensified Target (SIT) detector with the Optical Multichannel Analyzer (OMA),[26] a photomultiplier tube (RCA P28) was used. In this case the signal was transferred to a microamplifier unit. In both of the above cases, the output was monitored on a strip chart recorder. In the first combination, the SIT detector had a photocathode stage prior to its silicon target; a fiber optic faceplate (scintillator) was attached to this photocathode. This extends the response of the detector below 3000 Å and

close to the UV range (i.e., covers the Hg-resonance line of 2536 Å). This response was tested with the mercury hollow cathode lamp. The advantages of the SIT detector are the measurement of intensities at closely spaced wavelengths, i.e., line and background, and a substantial increase in the number of wavelengths that can be monitored. The dispersion of this Jarrel Ash monochromator is 16 Å/mm, and the width of the target on the detector is 12.7 mm. At the proper operating frame voltage (9 kV), a spectral range of ∿203 Å is covered on the oscilloscope screen. The sensitivity of a photomultiplier is normally higher than that of this detector. In the case of the photomultiplier, however, the signal-to-noise ratio is lower than with the SIT detector-OMA system. This SIT-OMA combination allows accumulation of the signal in the OMA unit (signal averaging technique) and results in a high signal-to-noise ratio.

In addition to the calibrant type of materials (i.e., lead, PbO, HgI_2) tested in this apparatus, a coal ash sample was also examined for any lead release. The experimental procedure in conducting a typical run or calibration was similar to that described for the alkali metal release studies.

RESULTS AND DISCUSSION

Among the combinations mentioned in the previous section, the largest calibration signal output for lead was obtained using the SIT detector-OMA unit. Such a calibration signal output illustrates the extent of the lead detection by this apparatus, as shown in Figure 16. The background level of this signal is obviously far from ideal. A similar signal was obtained when lead was used instead of PbO as the calibrant material, and also when the carrier gas was reducing (i.e., 22.1% H_2/19.4% CO/18.2% CO_2//N_2) instead of oxidizing, as illustrated in Figure 16.

The total amount of equivalent lead (185.6 µg) used for the calibration and the measured area (52.4 cm^2) under the resulting curve above the base line give a factor of 3.54 µg of Pb/cm^2. The area of 1 cm^2 is shown to scale on Figure 16. This area of 1 cm^2 corresponds

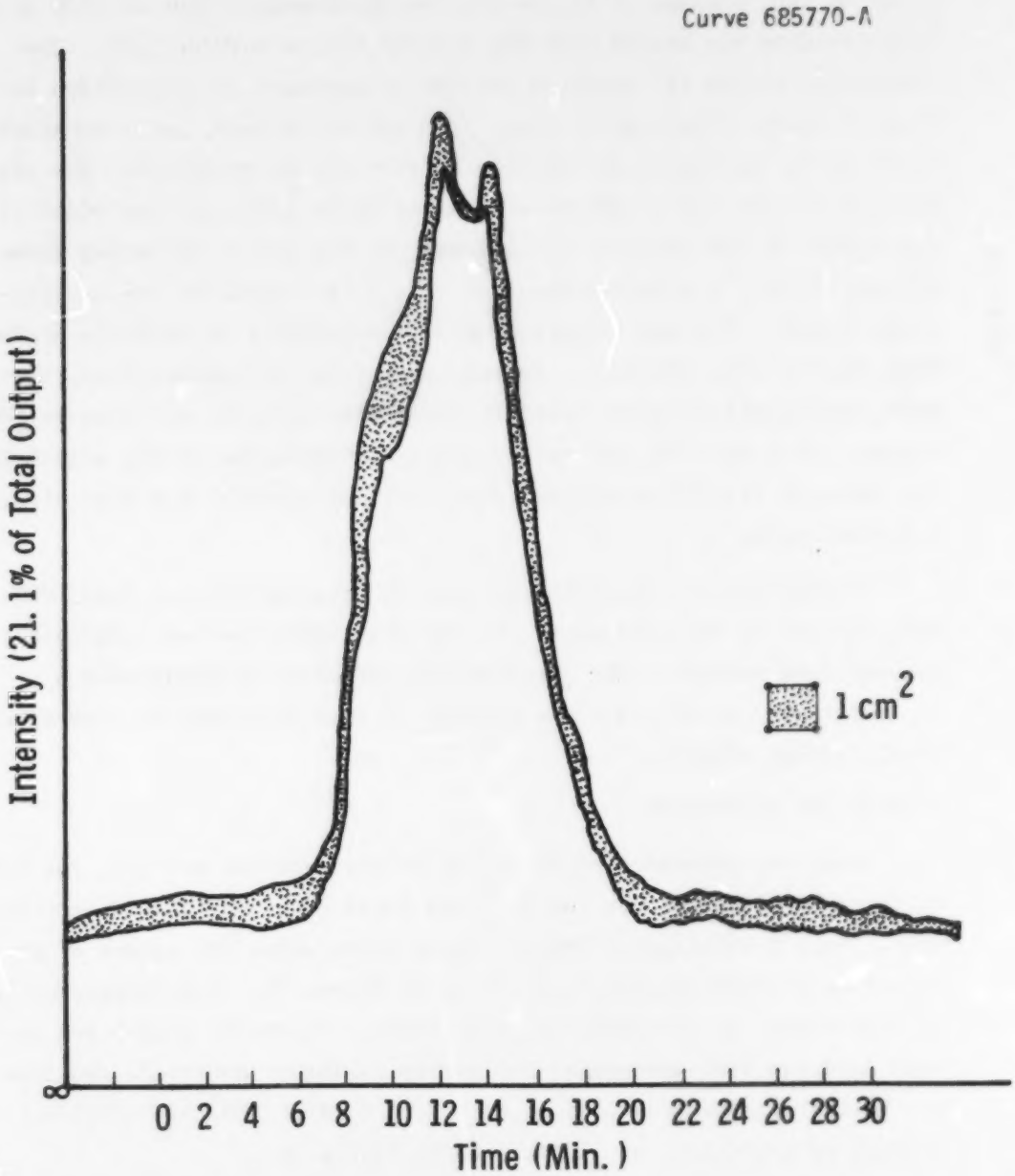

Figure 16. Total Signal Output of the Flame Emission Spectrum of Pb from 0.200 mg of PbO (i.e; ∿185.6 µg of Pb) (Resonance Line: 4059°A; Oxidizing Carrier Gas (19.8% CO_2/2.2% O_2//N_2 at 75 cc/min)

to 0.0155 division on the planimeter that was used for the area measurements. This is barely measurable with the planimeter. The observed fluctuations in the ordinate (intensity), however, do not justify more accurate means for the measurement of the area of the signal. In order to cover the low predicted range of the total lead release (i.e., 0.05–0.5 μg) from the sample volume that can be accommodated inside the nickel boat, the total area under the curve of Figure 16 should represent approximately less than 0.262 μg of lead; that is, an improvement by a factor of at least 708 (185.6/0.262) in the signal output is required. This allows a factor of ∿10 over the limit of detectability (i.e., twice the maximum variation of the background intensity). In practice, this expected minimum release (∿0.05 μg) will be the cumulative amount over a period of time; thus, another factor of approximately 10 may be needed for the accuracy required to establish the cumulative lead release curves.

This total improvement will yield a signal output comparable to that of sodium. The expected improvement in the best of the presently attainable signal outputs (Figure 16) from any changes in the monochromator (i.e., grating, slit width, etc.) will be minimal. The complete absence of any signal for lead when 100 mg of coal ash sample were slowly heated to 1323 K confirmed the result of Figure 16. The total amount of lead in this sample was 6.5 μg.* Hence, even in the unlikely situation of total lead release, this amount could have gone undetected.

Mercury was tested using HgI_2 as the calibrant material; the intensity of two mercury lines (2536 Å and 3650 Å) was followed as a function of time and flame position. The vapors of mercury were slowly generated at low temperatures (323–473 K) from samples of solid HgI_2. In no case was a calibration emission spectrum observed. The performance of the optical and detection systems was tested with the mercury hollow cathode lamp and was found satisfactory. The absence of any mercury flame emission spectrum during calibration

*Atomic absorption analysis of digested solution of the coal ash sample.

and the aforementioned lower flame emission sensitivity for mercury than lead did not justify any additional tests for the toxic mercury trace release. A total improvement by a factor of $\sim 10^6$ in the signal output of Figure 16 is estimated to be needed in order to be able to monitor continuously the release of mercury from the feed materials of the fluidized-bed combustor. Similarly, beryllium was not examined because its total content in the coals is reported as low as its optical emission spectroscopic detection limit.

In conclusion, the results of the tests and the available information in the literature show that the original objective - that is, the continuous monitoring of the toxic trace element release from the feed materials of the coal combustor process - cannot be accomplished using the flame emission spectrophotometric apparatus.

To achieve this objective, alternative methods and high-temperature sampling techniques must be developed. The use of atomic absorption, microwave excitation emission, and X-ray fluorescence techniques will not be adequate to monitor continuously the small releasable portion of the trace elements under the conditions of the coal combustor. Some recent determinations of the metallic elemental concentrations of heated (613-1523 K) coal ash samples in oxidizing atmospheres reveal, indeed, that any release would have been within the estimated precision of these techniques.[27,28] A reasonable approach may be the determination of a total trace element release (vapors and entrained particulates) through an analysis of condensates collected at selected time intervals. This analysis may be performed using the spark source mass spectrometric technique. Neutron activation analysis will be suitable for mercury if its constituents in the deposits are volatile under the spark source mass spectrometric conditions. The reported sensitivity in the nuclear reaction $^{202}Hg\ (n,\gamma)\ ^{203}Hg$ is 1×10^{-4} μg, as defined for 1000 disintegrations/minute of activation product after irradiation in a flux of 10^{14} neutrons/cm^2/s to saturation.[29]

SECTION 7

REFERENCES

1. Magee, E. M., H. J. Hall, and G. M. Varga, Jr., "Potential Pollutants in Fossil Fuels," Report to EPA, ESSO R&E Co., June 1973, Contract 68-02-0629, NTIS PB 225 039.

2. Joensuu, O. I., "Fossil Fuels as a Source of Mercury Pollution," Science 172, 1972, 1027-28.

3. Headlee, A. J. W., and R. G. Hunter, "The Inorganic Elements in the Coals," West Virginia Geological Survey, Vol. XIIIA, Morgantown, 1955.

4. Ruch, R. R., H. J. Gluskoter, and N. F. Shimp, "Occurrence and Distribution of Potentially Volatile Trace Elements in Coal," Report to EPA, Illinois State Geological Survey, July 1974, EPA 650/2-74-054, NTIS PB 238 091.

5. Page, C. L., et al., "Analysis of Coal and Overburden at Four Corners," Westinghouse Research and Development Center, December 13, 1973, Research Memo 73-7P4-ACHEJ-M2.

6. Hoke, R., "Emissions from Pressurized Fluidized Bed Combustion," Exxon R&E, Proceedings of the Fourth International Conference on Fluidized Bed Combustion. The Mitre Corporation, McLean, Virginia December 1975.

7. Swift, W. M., G. J. Vogel, A. F. Panek, and A. A. Jonke, "Trace Element Mass Balances around a Bench-Scale Combustor," Argonne National Laboratories., Proceedings of the Fourth International Conference on Fluidized Bed Combustion, The Mitre Corporation, McLean, Virginia, December 1975.

8. Knapp, N., Personal Communication, 1976.

9. Harvey, R. D., "Petrographic and Mineralogical Characteristics of Carbonate Rocks Related to Sulfur Dioxide Sorption in Flue Gases," Report to EPA, Illionois Geological Survey, July 1971, Contract CPA 22-69-65.

10. Unpublished Westinghouse Data.

11. O'Neill, E. P., D. L. Keairns, and M. A. Alvin, "Sorbent Selection for the CAFB Residual Oil Gasification Demonstration Plants," Westinghouse Research Laboratory, March 1977, EPA 600/7-77-029.

12. Private Communication, U. S. Geological Survey, Columbus, Ohio.

13. Liebermann, R. W., "Equilibrium and Thermodynamic Properties of Complex Chemical Mixtures," Westinghouse Research and Development Center, Pittsburgh, Pa., 1970.

14. Duffin, R. J., E. L. Peterson, and C. Zener, Geometric Programming, New York: John Wiley and Sons, 1967.

15. Chase, M. W., J. L. Curnutt, H. Prophet, R. A. McDonald, and A. N. Syverud, JANAF Thermochemical Tables. Journal of Physical and Chemical Reference Data, National Bureau of Standards, 2nd edition, and 1974-1975 supplements.

16. Hertzberg, G., Molecular Spectra and Molecular Structure I, II, III, New York: D. Van Nostrand Co., Inc., 1966.

17. Glassner, A., The Thermochemical Properties of the Oxides, Fluorides and Chlorides to 2500 K, Argonne National Laboratory, Argonne, Illinois, 1957, ANL-5750.

18. Barin, J. and O. Knacke, Thermochemical Properties of Inorganic Substances, Berlin: Springer-Verlag, 1973.

19. Oppermann, Von H., Fur Anorzanische und Allgemeine Chemie, Band 359, 52, 1968.

20. Krasnor, K. S., Handbook: Molecular Constants of Inorganic Compound, Khimiya, 1968.

21. National Bureau of Standards, Selected Values of Chemical Thermodynamic Properties, 1968, NBS TN 270-3.

22. Feber, R. C., Heats of Dissociation of Gaseous Halide, Los Alamos Scientific Laboratory, N. M., 1965, LA-3164, TSC-4, Chemistry TID-4500 (40th ed.).

23. Shick, H. L., Thermodynamics of Certain Refractory Compounds New York Academic Press, 1966.

24. Klein, D. H., W. Fulkerson, et al., "Pathways of Thirty-seven Trace Elements through a Coal-Fired Power Plant," Env. Sci. Technol. 9, 1975, p. 973.

25. Babu, S. P., Ed., "Trace Elements in Fuel," Advances in Chemistry Series, 141 (1975), p. 40, 45, 51.

26. Yannopoulos, L. N., et al., "Experimental Determination of Alkali Impurity Release from Various Dolomites," Combustion and Flame, 30, 1977, p. 61-69.

27. Vogel, G. J. et al., "A Development Program on Pressurized Fluidized Bed Combustion," Report to ERDA, EPA, Argonne National Laboratory, Argonne, Illinois, October-December, 1975, ANL/ES-CEN-1014.

28. Vogel, G. J., et al., "A Development Program on Pressurized Fluidized Bed Combustion," Report to ERDA, EPA, Argonne National Laboratory, Argonne, Illinois, January-March, 1976, ANL/ES-CEN-1015.

29. Meinke W. and B. Scribner Eds., Symposium on Trace Characterization, NBS Monograph 100, National Bureau of Standards, Washington, D. C., 1966.

30. Archer, D. H., et al., "Evaluation of the Fluidized-Bed Combustion Process," Vols. I-III, Report to EPA, Westinghouse Research and Development Center, Pittsburgh, Pa., November, 1971, Contract 76-9, NTIS PB 211-494, 212-960, 213-152.

31. Keairns, D. L., et al., "Evaluation of the Pressurized Fluidized-Bed Combustion Process - Pressurized Fluidized-Bed Combustion Process Development and Evaluation," Vols. I and II; "Pressurized Fluidized-Bed Boiler Development Plant Design," Vol. III, Report to EPA, Westinghouse Research and Development Center, Pittsburgh, Pa., December 1973, EPA 650/2-73-048 a, b, and c, NTIS Numbers 231-162, 231-163, 232-433.

32. Keairns, D. L., et al., "Pressurized Fluidized-Bed Coal Combustion Development," Report to EPA, Westinghouse Research and Development Center, Pittsburgh, Pa., September 1975, EPA 650/2-75-027c, NTIS PB 246-116.

33. Newby, R. A., and D. L. Keairns, "Alternatives to Calcium-Based SO_2 Sorbents for Fluidized-Bed Combustion: Conceptual Evaluation," Report to EPA, Westinghouse Research and Development Center, Pittsburgh, Pa., January 1978, EPA-600/7-78-005.

34. Newby, R. A., S. Katta, and D. L. Keairns, "Calcium-Based Sorbent Regeneration for Fluidized-Bed Combustion: Engineering Evaluation," Report to EPA, Westinghouse Research and Development Center, Pittsburgh, Pa., March 1978, EPA-600/7-78-039.

35. Sun, C. C., et al., Disposal of Solid Residue from Fluidized-Bed Combustion: Engineering and Laboratory Studies, Report to EPA, Westinghouse Research and Development Center, Pittsburgh, Pa., March 1978, EPA 600/7-78-049.

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APPENDIX A

CALCULATED PARTIAL PRESSURES OF GASEOUS TRACE COMPOUNDS AND MOLES OF TRACE-SOLIDS PRODUCED AT EQUILIBRIUM FOR HIGH COAL-HIGH DOLOMITE SYSTEMS AT 90 PERCENT SULFUR REMOVAL IN 0, 100, AND 300 PERCENT EXCESS AIR.

TABLE A1. HF

90% S Removal — 10% Excess Air

Species Name HF — PRESSURES

TEMP. K	.1500+02 ATM	.1000+02 ATM	.5000+01 ATM	.1000+01 ATM
.3000+03	.2365-06	.1976-06	.9892-07	.1976-07
.4000+03	.5553-05	.3702-05	.1851-05	.3629-06
.5000+03	.3060-04	.2041-04	.1022-04	.2065-05
.6000+03	.8502-04	.5765-04	.3017-04	.7436-05
.7000+03	.1557-03	.1065-03	.5519-04	.1150-04
.8000+03	.1737-03	.1160-03	.5810-04	.1164-04
.9000+03	.1746-03	.1164-03	.5821-04	.1164-04
.1000+04	.1746-03	.1164-03	.5821-04	.1164-04
.1100+04	.1746-03	.1164-03	.5821-04	.1164-04
.1200+04	.1746-03	.1164-03	.5818-04	.1162-04

100% Excess Air

Species Name HF — PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.1668-06	.1112-06	.5561-07	.1112-07
.4000+03	.3125-05	.2083-05	.1042-05	.2083-06
.5000+03	.1724-04	.1150-04	.5764-05	.1174-05
.6000+03	.4910-04	.3263-04	.1793-04	.4619-05
.7000+03	.9077-04	.6176-04	.3170-04	.6505-05
.8000+03	.9730-04	.6538-04	.3273-04	.7086-05
.9000+03	.9829-04	.6553-04	.3276-04	.6557-05
.1000+04	.9829-04	.6553-04	.3276-04	.6553-05
.1100+04	.9829-04	.6553-04	.3276-04	.6553-05
.1200+04	.9829-04	.6553-04	.3275-04	.6538-05

300% Excess Air

Species Name Hf — PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.8462-07	.5641-07	.2821-07	.5642-08
.4000+03	.1585-05	.1057-05	.5284-06	.1057-06
.5000+03	.8758-05	.5847-05	.2937-05	.6082-06
.6000+03	.2617-04	.1821-04	.1001-04	.2617-05
.7000+03	.4755-04	.3214-04	.1632-04	.3312-05
.8000+03	.4977-04	.3320-04	.1662-04	.3324-05
.9000+03	.4986-04	.3324-04	.1662-04	.3324-05
.1000+04	.4986-04	.3324-04	.1662-04	.3324-05
.1100+04	.4986-04	.3324-04	.1662-04	.3324-05
.1200+04	.4986-04	.3324-04	.1661-04	.3312-05

System: C-H-N-O-S-Cl-K-Na-F

TABLE A2. KF

90% S Removal 10% Excess Air

Species Name KF G PRESSURES

TEMP. K

	.1500+02 ATM	.1000+02 ATM	.5000+01 ATM	.1000+01 ATM
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.3819-36	.3118-36	.2205-36	.9881-37
.5000+03	.7896-28	.6452-28	.4574-28	.2091-28
.6000+03	.2380-22	.2028-22	.1608-22	.1259-22
.7000+03	.2590-18	.2510-18	.2441-18	.2412-18
.8000+03	.3191-15	.3184-15	.3198-15	.3324-15
.9000+03	.8018-13	.8179-13	.8546-13	.9973-13
.1000+04	.7287-11	.7661-11	.8445-11	.1116-10
.1100+04	.3270-09	.3522-09	.4026-09	.5560-09
.1200+04	.8099-08	.8762-08	.9955-08	.1288-07

100% Excess Air

Species Name KF G PRESSURES

TEMP. K

	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.2865-36	.2339-36	.1654-36	.7398-37
.5000+03	.5971-28	.4851-28	.3447-28	.1602-28
.6000+03	.1904-22	.1622-22	.1297-22	.1272-22
.7000+03	.2432-18	.2443-18	.2411-18	.2394-18
.8000+03	.3126-15	.3119-15	.3126-15	.3449-15
.9000+03	.7595-13	.7676-13	.7865-13	.8640-13
.1000+04	.6338-11	.6548-11	.6999-11	.8640-11
.1100+04	.2891-09	.2744-09	.3058-09	.4022-09
.1200+04	.6007-08	.6417-08	.7153-08	.9019-08

300% Excess Air

Species Name KF G PRESSURES

TEMP. K

	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.2041-36	.1666-36	.1178-36	.5269-37
.5000+03	.4238-28	.3472-28	.2478-28	.1193-28
.6000+03	.1537-22	.1400-22	.1277-22	.1331-22
.7000+03	.2423-18	.2408-18	.2395-18	.2385-18
.8000+03	.3107-15	.3103-15	.3108-15	.3158-15
.9000+03	.7512-13	.7582-13	.7742-13	.8394-13
.1000+04	.6162-11	.6339-11	.6722-11	.8126-11
.1100+04	.2454-09	.2584-09	.2848-09	.3624-09
.1200+04	.5498-08	.5816-08	.6374-08	.7960-08

System: C-H-N-O-S-Cl-K-Na-F

TABLE A3. NaF

90% S Removal — 10% Excess Air

Species Name NaF — G PRESSURES

TEMP. K	.1500+02 ATM	.1000+02 ATM	.5000+01 ATM	.1000+01 ATM
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.8556-29	.6991-29	.4956-29	.2265-29
.6000+03	.3478-23	.2962-23	.2348-23	.1840-23
.7000+03	.4443-19	.4307-19	.4189-19	.4138-19
.8000+03	.6161-16	.6169-16	.6194-16	.6440-16
.9000+03	.1806-13	.1842-13	.1925-13	.2246-13
.1000+04	.1885-11	.1982-11	.2185-11	.2886-11
.1100+04	.9429-10	.1015-09	.1161-09	.1603-09
.1200+04	.2405-08	.2602-08	.2956-08	.3826-08

100% Excess Air

Species Name NaF — G PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.6427-29	.5256-29	.3735-29	.1736-29
.6000+03	.2781-23	.2430-23	.2041-23	.1858-23
.7000+03	.4258-19	.4192-19	.4126-19	.4107-19
.8000+03	.6056-16	.6043-16	.6056-16	.6681-16
.9000+03	.1710-13	.1729-13	.1771-13	.1946-13
.1000+04	.1640-11	.1634-11	.1811-11	.2235-11
.1100+04	.7470-10	.7913-10	.8817-10	.1160-09
.1200+04	.1784-08	.1905-08	.2124-08	.2679-08

300% Excess Air

Species Name NaF — G PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.4592-29	.3762-29	.2686-29	.1293-29
.6000+03	.2245-23	.2045-23	.1866-23	.1944-23
.7000+03	.4157-19	.4131-19	.4108-19	.4092-19
.8000+03	.6019-16	.6011-16	.6022-16	.6118-16
.9000+03	.1692-13	.1707-13	.1743-13	.1890-13
.1000+04	.1594-11	.1640-11	.1739-11	.2102-11
.1100+04	.7075-10	.7451-10	.8212-10	.1045-09
.1200+04	.1633-08	.1727-08	.1893-08	.2364-08

System: C-H-N-O-S-Cl-K-Na-F

TABLE A4. SO_2F_2

90% S Removal — 10% Excess Air

Species Name SO_2F_2 S PRESSURES

TEMP. K	.1500+02 ATM	.1000+02 ATM	.5000+01 ATM	.1000+01 ATM
.3000+03	.8719-04	.5813-04	.2906-04	.5813-05
.4000+03	.8456-04	.5637-04	.2819-04	.5641-05
.5000+03	.7204-04	.4802-04	.2400-04	.4790-05
.6000+03	.4492-04	.2939-04	.1402-04	.2104-05
.7000+03	.9480-05	.4968-05	.1514-05	.7301-07
.8000+03	.4906-06	.2205-06	.5508-07	.2051-08
.9000+03	.2933-07	.1253-07	.2872-08	.8435-10
.1000+04	.2248-08	.9042-09	.1860-09	.4263-11
.1100+04	.2055-09	.7874-10	.1506-10	.3158-12
.1200+04	.2440-10	.9265-11	.1791-11	.4248-13

100% Excess Air

Species Name SO_2F_2 S PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.4906-04	.3271-04	.1635-04	.3271-05
.4000+03	.4759-04	.3172-04	.1586-04	.3173-05
.5000+03	.4053-04	.2701-04	.1350-04	.2690-05
.6000+03	.2480-04	.1595-04	.7392-05	.9676-06
.7000+03	.5763-05	.1875-05	.5379-06	.2390-07
.8000+03	.1634-05	.7292-07	.1831-07	.8271-09
.9000+03	.1038-07	.4512-08	.1074-08	.3561-10
.1000+04	.9417-09	.3922-09	.8581-10	.2252-11
.1100+04	.1077-09	.4108-10	.8273-11	.1912-12
.1200+04	.1405-10	.5472-11	.1099-11	.2741-13

300% Excess Air

Species Name SO_2F_2 S PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.2483-04	.1659-04	.8296-05	.1659-05
.4000+03	.2414-04	.1609-04	.8046-05	.1609-05
.5000+03	.2055-04	.1370-04	.6842-05	.1358-05
.6000+03	.1184-04	.7517-05	.3303-05	.3537-06
.7000+03	.1153-05	.5494-06	.1478-06	.6224-08
.8000+03	.4258-07	.1915-07	.4761-08	.1834-09
.9000+03	.2726-08	.1190-08	.2853-09	.9707-11
.1000+04	.2564-09	.1077-09	.2393-10	.6551-12
.1100+04	.2975-10	.1192-10	.2453-11	.6059-13
.1200+04	.4315-11	.1713-11	.3557-12	.9005-14

System: C-H-N-O-S-Cl-K-Na-F

TABLE A5. $BeSO_4$

90% S Removal — 10% Excess Air

Species Name $BeSO_4$ (s) — Moles

TEMP. K	.1500+02 ATM	.1000+02 ATM	.5000+01 ATM	.1000+01 ATM
.3000+03	.3916-04	.3915-04	.3915-04	.3916-04
.4000+03	.3916-04	.3916-04	.3915-04	.3916-04
.5000+03	.3918-04	.3917-04	.3917-04	.3916-04
.6000+03	.3686-04	.0000	.0000	.0000
.7000+03	.0000	.0000	.0000	.0000
.8000+03	.0000	.0000	.0000	.0000
.9000+03	.0000	.0000	.0000	.0000
.1000+04	.0000	.0000	.0000	.0000
.1100+04	.0000	.0000	.0000	.0000
.1200+04	.0000	.0000	.0000	.0000

100% Excess Air

Species Name $BeSO_4$ (s) — Moles

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.3918-04	.3918-04	.3918-04	.3918-04
.4000+03	.3918-04	.3918-04	.3918-04	.3918-04
.5000+03	.3918-04	.3918-04	.3919-04	.3919-04
.6000+03	.3834-04	.0000	.0000	.0000
.7000+03	.0000	.0000	.0000	.0000
.8000+03	.0000	.0000	.0000	.0000
.9000+03	.0000	.0000	.0000	.0000
.1000+04	.0000	.0000	.0000	.0000
.1100+04	.0000	.0000	.0000	.0000
.1200+04	.0000	.0000	.0000	.0000

300% Excess Air — Moles

Species Name $BeSO_4$ (s)

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	[illegible]	[illegible]	.3920-04	.3921-04
.4000+03	[illegible]	[illegible]	.3920-04	.3921-04
.5000+03	[illegible]	[illegible]	.3920-04	.3920-04
.6000+03	.3731-04	.0000	.0000	.2503-04
.7000+03	.0000	.0000	.0000	.0000
.8000+03	.0000	.0000	.0000	.0000
.9000+03	.0000	.0000	.0000	.0000
.1000+04	.0000	.0000	.0000	.0000
.1100+04	.0000	.0000	.0000	.0000
.1200+04	.0000	.0000	.0000	.0000

System: C-H-N-O-S-Cl-K-Na-Be

TABLE A6. $Be(OH)_2$

90% S Removal

10% Excess Air

Species Name $Be(OH)_2$ PRESSURES

TEMP. K	.1500+02 ATM	.1000+02 ATM	.5000+01 ATM	.1000+01 ATM
.3000+03	.6068-20	.4477-20	.2662-20	.7961-21
.4000+03	.1297-12	.9570-13	.5690-13	.1711-13
.5000+03	.3188-08	.2354-08	.1403-08	.4294-09
.6000+03	.2964-05	.2301-05	.1570-05	.9502-06
.7000+03	.1536-04	.1024-04	.5121-05	.1024-05
.8000+03	.1536-04	.1024-04	.5120-05	.1024-05
.9000+03	.1536-04	.1024-04	.5119-05	.1024-05
.1000+04	.1536-04	.1024-04	.5119-05	.1024-05
.1100+04	.1536-04	.1024-04	.5119-05	.1024-05
.1200+04	.1536-04	.1024-04	.5122-05	.1024-05

100% Excess Air

Species Name $Be(OH)_2$ PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.6547-20	.4830-20	.2872-20	.8589-21
.4000+03	.1339-12	.1032-12	.6139-13	.1836-13
.5000+03	.3444-08	.2545-08	.1521-08	.4736-09
.6000+03	.7452-05	.5763-05	.3423-05	.5750-06
.7000+03	.8624-05	.5750-05	.2875-05	.5750-06
.8000+03	.8624-05	.5750-05	.2875-05	.6006-06
.9000+03	.8632-05	.5766-05	.2883-05	.5765-06
.1000+04	.8648-05	.5765-05	.2883-05	.5765-06
.1100+04	.8648-05	.5765-05	.2877-05	.5755-06
.1200+04	.8651-05	.5768-05	.2883-05	.5766-06

300% Excess Air

Species Name $Be(OH)_2$ PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.5146-20	.3797-20	.2257-20	.6754-21
.4000+03	.1100-12	.8119-13	.4827-13	.1444-13
.5000+03	.2717-08	.2011-08	.1206-08	.3904-09
.6000+03	.2559-05	.2064-05	.1462-05	.2919-06
.7000+03	.4363-05	.2915-05	.1454-05	.2919-06
.8000+03	.4379-05	.2919-05	.1461-05	.2922-06
.9000+03	.4383-05	.2923-05	.1461-05	.2923-06
.1000+04	.4384-05	.2923-05	.1462-05	.2923-06
.1100+04	.4385-05	.2923-05	.1462-05	.2923-06
.1200+04	.4385-05	.2923-05	.1457-05	.2916-06

System: C-H-N-O-S-Cl-K-Na-Be

TABLE A7. $HgCl_2$

90% S Removal 10% Excess Air

Species Name $HgCl_2$ G PRESSURES

TEMP. K

	.1500+02 ATM	.1000+02 ATM	.5000+01 ATM	.1000+01 ATM
.3000+03	.7636-07	.5090-07	.2545-07	.5090-09
.4000+03	.7636-07	.5090-07	.2545-07	.5090-08
.5000+03	.7635-07	.5090-07	.2545-07	.5090-08
.6000+03	.8040-07	.5360-07	.2680-07	.4411-08
.7000+03	.7467-07	.4980-07	.2483-07	.4978-08
.8000+03	.7464-07	.4978-07	.2489-07	.4879-08
.9000+03	.7467-07	.4978-07	.2338-07	.2025-08
.1000+04	.3684-07	.1929-07	.4444-08	.9177-10
.1100+04	.4174-08	.1557-08	.2795-09	.4192-11
.1200+04	.3581-09	.1238-09	.1855-10	.1052-12

100% Excess Air

Species Name $HgCl_2$ G PRESSURES

TEMP. K

	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.3529-07	.2353-07	.1177-07	.2941-08
.4000+03	.3559-07	.2382-07	.1194-07	.2955-08
.5000+03	.3700-07	.2474-07	.1804-07	.2989-08
.6000+03	.3824-07	.2760-07	.1380-07	.2763-08
.7000+03	.4288-07	.2770-07	.1387-07	.2780-08
.8000+03	.4287-07	.2780-07	.1427-07	.2872-08
.9000+03	.3974-07	.2761-07	.1283-07	.1195-08
.1000+04	.2259-07	.1036-07	.2534-08	.5674-10
.1100+04	.2490-08	.9580-09	.1613-09	.2477-11
.1200+04	.2311-09	.7934-10	.8872-11	.4881-13

300% Excess Air

Species Name $HgCl_2$ G PRESSURES

TEMP. K

	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.2516-07	.1677-07	.8385-08	.1526-08
.4000+03	.2516-07	.1435-07	.7177-08	.1528-08
.5000+03	.2516-07	.1497-07	.7691-08	.1535-08
.6000+03	.2319-07	.1520-07	.8600-08	.1348-08
.7000+03	.2509-07	.1348-07	.8362-08	.1348-08
.8000+03	.2023-07	.1348-07	.8746-08	.1350-08
.9000+03	.2025-07	.1490-07	.8749-08	.4890-09
.1000+04	.1023-07	.4262-08	.1003-08	.1924-10
.1100+04	.8468-09	.3150-09	.5628-10	.7362-12
.1200+04	.6493-10	.2128-10	.2663-11	.7401-14

System: C-H-N-O-S-Cl-K-Na-Hg

TABLE A8. Hg

90% S Removal

10% Excess Air

Species Name Hg

PRESSURES

TEMP. K	.1500+02 ATM	.1000+02 ATM	.5000+01 ATM	.1000+01 ATM
.3000+03	.7369-35	.7375-35	.7396-35	.7422-35
.4000+03	.8925-26	.9051-26	.9304-26	.1014-25
.5000+03	.4162-20	.4483-20	.5172-20	.7837-20
.6000+03	.6375-16	.7473-16	.9940-16	.1671-15
.7000+03	.9310-13	.1128-12	.1575-12	.3444-12
.8000+03	.2608-10	.3188-10	.4488-10	.9778-10
.9000+03	.2133-08	.2609-08	.3459-08	.3342-08
.1000+04	.3575-07	.3438-07	.2239-07	.5197-08
.1100+04	.7294-07	.5020-07	.2586-07	.5041-08
.1200+04	.7559-07	.5085-07	.2576-07	.5412-08

100% Excess Air

Species Name Hg

PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.6038-35	.6042-35	.6049-35	.7586-35
.4000+03	.7122-26	.7201-26	.7396-26	.9665-26
.5000+03	.2885-20	.3054-20	.4120-20	.5592-20
.6000+03	.3230-16	.3997-16	.5111-16	.9752-16
.7000+03	.4991-13	.5759-13	.7969-13	.1685-12
.8000+03	.1315-10	.1579-10	.2239-10	.4868-10
.9000+03	.9651-09	.1262-08	.1640-08	.1701-08
.1000+04	.1894-07	.1671-07	.1124-07	.2779-08
.1100+04	.3768-07	.2822-07	.1300-07	.2695-08
.1200+04	.4339-07	.2939-07	.1156-07	.2759-08

300% Excess Air

Species Name Hg

PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.8483-35	.8487-35	.8495-35	.7752-35
.4000+03	.9814-26	.9869-26	.9821-26	.9688-26
.5000+03	.3689-20	.3857-20	.3905-20	.5191-20
.6000+03	.3408-16	.3809-16	.4179-16	.7977-16
.7000+03	.4745-13	.4577-13	.7747-13	.1332-12
.8000+03	.1076-10	.1247-10	.1746-10	.3883-10
.9000+03	.8141-09	.1096-08	.1393-08	.1128-08
.1000+04	.1397-07	.1063-07	.7080-08	.1539-08
.1100+04	.2095-07	.1447-07	.7571-08	.1525-08
.1200+04	.2179-07	.1479-07	.7384-08	.1404-08

System: C-H-N-O-S-Cl-K-Na-Hg

TABLE A9. HgO

90% S Removal

10% Excess Air

Species Name HgO C

TEMP. K

	.1500+02 ATM	.1000+02 ATM	.5000+01 ATM	.1000+01 ATM
.3000+03	.1[illegible]-33	.6932-34	.6326-34	.2843-34
.4000+03	.1[illegible]-25	.1543-25	.1121-25	.5[illegible]5-26
.5000+03	.2[illegible]4-20	.2335-20	.1505-20	.1[illegible]1-20
.6000+03	.1[illegible]8-16	.1759-16	.1[illegible]5-16	.1244-16
.7000+03	.1[illegible]-13	.1[illegible]1-13	.1483-[illegible]	.1451-13
.8000+03	.2771-11	.[illegible]765-11	.2752-11	.2682-11
.9000+03	.1[illegible]-09	.1[illegible]-09	.1518-09	.6561-10
.1000+04	.2[illegible]-08	.1[illegible]-08	.7510-09	.7797-10
.1100+04	.3[illegible]-08	.1[illegible]-08	.[illegible]51-09	.[illegible]060-10
.1200+04	.2[illegible]-08	.1[illegible]-08	.5749-09	.5404-10

100% Excess Air

Species Name HgO C

TEMP. K

	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.1852-33	.1513-33	.1071-33	.6009-34
.4000+03	.3074-25	.2538-25	.1873-25	.1077-25
.5000+03	.3804-20	.3237-20	.2376-20	.1904-20
.6000+03	.1924-16	.1644-16	.1758-16	.1500-16
.7000+03	.1648-13	.1[illegible]4-13	.1550-13	.1468-13
.8000+03	.2879-11	.2829-11	.2831-11	.2759-11
.9000+03	.1520-09	.1[illegible]7-09	.1487-09	.6896-10
.1000+04	.2271-08	.1[illegible]6-08	.7781-09	.8804-10
.1100+04	.3621-08	.2057-08	.7212-09	.6687-10
.1200+04	.3401-08	.1315-08	.5322-09	.5683-10

300% Excess Air

Species Name HgO C PRESSURES

TEMP. K

	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.3171-33	.2591-33	.1834-33	.7485-34
.4000+03	.5163-25	.3636-25	.2613-25	.1316-25
.5000+03	.5927-20	.4536-20	.3624-20	.2154-20
.6000+03	.2474-16	.1961-16	.1752-16	.1495-16
.7000+03	.1949-13	.1535-13	.1836-13	.1412-13
.8000+03	.2876-11	.2724-11	.2686-11	.2681-11
.9000+03	.1558-09	.1713-09	.1545-09	.5570-10
.1000+04	.2042-08	.1269-08	.5974-09	.5809-10
.1100+04	.2453-08	.1383-08	.5113-09	.4611-10
.1200+04	.2119-08	.1174-08	.4146-09	.3524-10

System: C-H-N-O-S-Cl-K-Na-Hg

TABLE A10. Hg_2

90% S Removal

10% Excess Air

Species Name Hg_2 PRESSURES

TEMP. K	.1500+02 ATM	.1000+02 ATM	.5000+01 ATM	.1000+01 ATM
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.0000	.0000	.0000	.0000
.6000+03	.3675-34	.5050-34	.8935-34	.2525-33
.7000+03	.5093-28	.7479-28	.1459-27	.6975-27
.8000+03	.2874-23	.4293-23	.8505-23	.4022-22
.9000+03	.1477-19	.2210-19	.3885-19	.3627-19
.1000+04	.3346-17	.3094-17	.1313-17	.7073-19
.1100+04	.1164-16	.5513-17	.1463-17	.5558-19
.1200+04	.1072-16	.4853-17	.1245-17	.5497-19

100% Excess Air

Species Name Hg_2

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.0000	.0000	.0000	.0000
.6000+03	.9436-35	.1445-34	.2363-34	.8601-34
.7000+03	.1406-28	.1949-28	.3732-28	.1669-27
.8000+03	.7287-24	.1053-23	.2113-23	.1001-22
.9000+03	.3047-20	.5170-20	.8737-20	.9398-20
.1000+04	.9394-18	.7309-18	.3307-18	.2022-19
.1100+04	.3107-17	.1504-17	.3697-18	.1589-19
.1200+04	.3533-17	.1621-17	.2505-18	.1428-19

300% Excess Air

Species Name Hg_2 PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.0000	.0000	.0000	.0000
.6000+03	.1050-34	.9839-35	.1580-34	.5755-34
.7000+03	.1322-28	.1231-28	.3525-28	.1042-27
.8000+03	.4386-24	.6570-24	.1278-23	.6368-23
.9000+03	.2152-20	.3903-20	.6355-20	.4128-20
.1000+04	.5111-18	.2961-18	.1312-18	.6204-20
.1100+04	.9600-18	.4579-18	.1254-18	.5087-20
.1200+04	.8913-18	.4105-18	.1023-18	.3698-20

System: C-H-N-O-S-Cl-K-Na-Hg

TABLE A11. HgCl

90% S Removal — 10% Excess Air

Species Name HgCl — PRESSURES

TEMP. K	.1500+02 ATM	.1000+02 ATM	.5000+01 ATM	.1000+01 ATM
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.8445-31	.6944-31	.4978-31	.2324-31
.5000+03	.3084-25	.6850-25	.5202-25	.2864-25
.6000+03	.1269-20	.1122-20	.9150-21	.4813-21
.7000+03	.1446-17	.1300-17	.1086-17	.7179-18
.8000+03	.3151-15	.2845-15	.2387-15	.1557-15
.9000+03	.2087-13	.1885-13	.1487-13	.4302-14
.1000+04	.2939-12	.2086-12	.8078-13	.5593-14
.1100+04	.5165-12	.2617-12	.7958-13	.4303-14
.1200+04	.4523-12	.2182-12	.6009-13	.2074-14

100% Excess Air

Species Name HgCl — PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.5158-31	.4237-31	.3071-31	.1729-31
.5000+03	.4685-25	.3942-25	.3570-25	.1854-25
.6000+03	.8231-21	.6988-21	.4708-21	.2910-21
.7000+03	.7341-18	.5925-18	.5735-18	.3754-18
.8000+03	.1694-15	.1437-15	.1276-15	.8445-16
.9000+03	.1010-13	.9797-14	.7585-14	.2358-14
.1000+04	.1675-12	.1031-12	.4364-13	.3216-14
.1100+04	.2963-12	.1468-12	.4287-13	.2419-14
.1200+04	.2753-12	.1328-12	.2784-13	.1009-14

System: C-H-N-O-S-Cl-K-Na-Hg

TABLE A12. $PbCl_4$

90% S Removal

10% Excess Air

Species Name $PbCl_4$ C PRESSURES

TEMP. K	.1500+02 ATM	.1000+02 ATM	.5000+01 ATM	.1000+01 ATM
.3000+03	.1581-04	.1054-04	.5270-05	.1054-05
.4000+03	.1581-04	.1054-04	.5270-05	.1054-05
.5000+03	.1581-04	.1054-04	.5269-05	.1054-05
.6000+03	.1581-04	.1054-04	.5270-05	.1053-05
.7000+03	.1580-04	.1054-04	.5266-05	.1054-05
.8000+03	.1580-04	.1053-04	.5266-05	.1054-05
.9000+03	.1580-04	.1053-04	.5269-05	.1054-05
.1000+04	.1580-04	.1054-04	.5269-05	.1054-05
.1100+04	.1581-04	.1054-04	.5269-05	.1054-05
.1200+04	.1575-04	.1047-04	.5143-05	.3294-06

100% Excess Air

Species Name $PbCl_4$ C PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.8897-05	.5931-05	.2966-05	.5931-06
.4000+03	.8897-05	.5931-05	.2966-05	.5931-06
.5000+03	.8897-05	.5931-05	.2965-05	.5930-06
.6000+03	.8890-05	.5930-05	.2965-05	.5928-06
.7000+03	.8892-05	.5928-05	.2964-05	.5928-06
.8000+03	.8892-05	.5928-05	.2964-05	.5933-06
.9000+03	.8893-05	.5932-05	.2966-05	.5931-06
.1000+04	.8897-05	.5932-05	.2966-05	.5931-06
.1100+04	.8897-05	.5931-05	.2965-05	.5909-06
.1200+04	.8867-05	.5894-05	.2892-05	.1122-06

300% Excess Air

Species Name $PbCl_4$ C PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.4511-05	.3007-05	.1504-05	.3008-06
.4000+03	.4511-05	.3006-05	.1503-05	.3008-06
.5000+03	.4511-05	.3008-05	.1504-05	.3008-06
.6000+03	.4512-05	.3007-05	.1503-05	.3006-06
.7000+03	.4513-05	.3006-05	.1504-05	.3006-06
.8000+03	.4510-05	.3006-05	.1503-05	.3006-06
.9000+03	.4510-05	.3007-05	.1503-05	.3007-06
.1000+04	.4511-05	.3007-05	.1504-05	.3007-06
.1100+04	.4511-05	.3007-05	.1504-05	.2986-06
.1200+04	.4489-05	.2976-05	.1411-05	.5994-08

System: C-H-N-O-S-Cl-K-Na-Pb

TABLE A13. $PbCl_2$

90% S Removal — 10% Excess Air

Species Name $PbCl_2$ G PRESSURES

TEMP. K	.1500+02 ATM	.1000+02 ATM	.5000+01 ATM	.1000+01 ATM
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.8987-33	.9680-33	.1117-32	.1692-32
.6000+03	.1130-25	.1324-25	.1762-25	.3594-25
.7000+03	.2173-20	.2632-20	.3676-20	.8045-20
.8000+03	.2204-16	.2691-16	.3787-16	.8425-16
.9000+03	.2894-13	.3539-13	.5000-13	.1115-12
.1000+04	.8971-11	.1099-10	.1553-10	.3492-10
.1100+04	.9779-09	.1203-08	.1726-08	.4464-08
.1200+04	.5235-07	.6767-07	.1125-06	.2669-06

100% Excess Air

Species Name $PbCl_2$ G PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.7236-33	.7834-33	.8469-33	.1157-32
.6000+03	.6767-26	.7740-26	.9899-26	.1886-25
.7000+03	.1119-20	.1360-20	.1878-20	.3963-20
.8000+03	.1087-16	.1343-16	.1854-16	.4013-16
.9000+03	.1409-13	.1726-13	.2433-13	.5415-13
.1000+04	.4365-11	.5341-11	.7549-11	.1700-10
.1100+04	.4706-09	.5869-09	.8459-09	.2276-08
.1200+04	.2622-07	.3439-07	.5932-07	.9984-07

300% Excess Air

Species Name $PbCl_2$ G PRESSURES

TEMP. K	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.6897-33	.7243-33	.7964-33	.1061-32
.6000+03	.5989-26	.6792-26	.8579-26	.1603-25
.7000+03	.9411-21	.1126-20	.1537-20	.3275-20
.8000+03	.9567-17	.1109-16	.1546-16	.3451-16
.9000+03	.1163-13	.1419-13	.1998-13	.4446-13
.1000+04	.3588-11	.4390-11	.6208-11	.1408-10
.1100+04	.3950-09	.4889-09	.7162-09	.2190-08
.1200+04	.2373-07	.3257-07	.5150-07	.1790-07

System: C-H-N-O-S-Cl-K-Na-Pb

TABLE A14. PbO

90% S Removal

10% Excess Air

Species Name PbO C PRESSURES

TEMP. K

	.1500+02 ATM	.1000+02 ATM	.5000+01 ATM	.1000+01 ATM
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.0000	.0000	.0000	.0000
.6000+03	.0000	.0000	.0000	.9033-38
.7000+03	.1076-30	.1934-31	.5336-30	.5712-29
.8000+03	.4268-24	.7737-24	.2185-23	.2417-22
.9000+03	.5963-19	.1093-18	.3082-18	.3431-17
.1000+04	.7789-15	.1436-14	.4045-14	.4572-13
.1100+04	.1829-11	.3389-11	.9873-11	.1484-09
.1200+04	.1376-08	.2826-08	.1124-07	.4420-06

100% Excess Air

Species Name PbO C PRESSURES

TEMP. K

	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.0000	.0000	.0000	.0000
.6000+03	.0000	.0000	.0000	.9129-38
.7000+03	.1047-30	.1894-30	.5111-30	.5590-29
.8000+03	.3810-24	.7229-24	.1922-23	.2011-22
.9000+03	.5191-19	.9830-19	.2677-18	.2966-17
.1000+04	.6792-15	.1240-14	.3503-14	.3971-13
.1100+04	.1594-11	.2960-11	.8697-11	.1413-09
.1200+04	.1255-08	.2575-08	.1147-07	.3746-06

300% Excess Air

Species Name PbO C PRESSURES

TEMP. K

	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.0000	.0000	.0000	.0000
.6000+03	.0000	.0000	.0000	.1585-37
.7000+03	.1779-30	.3120-30	.8222-30	.8354-29
.8000+03	.7096-24	.1169-23	.3212-23	.3576-22
.9000+03	.8493-19	.1549-18	.4344-18	.4808-17
.1000+04	.1058-14	.2014-14	.5696-14	.6549-13
.1100+04	.2632-11	.4938-11	.1499-10	.3155-09
.1200+04	.2496-08	.5791-08	.3079-07	.2747-06

System: C-H-N-O-S-Cl-K-Na-Pb

TABLE A15. PbCl

90% S Removal

10% Excess Air

Species Name PbCl C PRESSURES

TEMP. K

	.1500+02 ATM	.1000+02 ATM	.5000+01 ATM	.1000+01 ATM
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.0000	.0000	.0000	.0000
.6000+03	.0000	.0000	.5224-37	.3405-36
.7000+03	.1359-29	.2218-29	.5173-29	.3748-28
.8000+03	.1441-23	.2361-23	.5623-23	.4171-22
.9000+03	.7109-19	.1179-18	.2796-18	.2083-17
.1000+04	.4016-15	.6664-15	.1585-14	.1194-13
.1100+04	.4721-12	.7887-12	.1918-11	.1788-10
.1200+04	.1911-09	.3446-09	.1053-08	.1521-07

100% Excess Air

Species Name PbCl C PRESSURES

TEMP. K

	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.0000	.0000	.0000	.0000
.6000+03	.0000	.0000	.0000	.1725-36
.7000+03	.6690-30	.1088-29	.2520-29	.1728-28
.8000+03	.6658-24	.1129-23	.2666-23	.1827-22
.9000+03	.7221-19	.5344-19	.1265-18	.9792-18
.1000+04	.1818-15	.3011-15	.7155-15	.5405-14
.1100+04	.2141-12	.3584-12	.8770-12	.8672-11
.1200+04	.9026-10	.1663-09	.5379-09	.5967-08

300% Excess Air

Species Name PbCl C PRESSURES

TEMP. K

	.1500+02	.1000+02	.5000+01	.1000+01
.3000+03	.0000	.0000	.0000	.0000
.4000+03	.0000	.0000	.0000	.0000
.5000+03	.0000	.0000	.0000	.0000
.6000+03	.0000	.0000	.3324-37	.1898-36
.7000+03	.7245-30	.1161-29	.2613-29	.1822-28
.8000+03	.7714-24	.1180-23	.2746-23	.2047-22
.9000+03	.3389-19	.5596-19	.1322-18	.9814-13
.1000+04	.1911-15	.3152-15	.7494-15	.5722-14
.1100+04	.2269-12	.3827-12	.9595-12	.1151-10
.1200+04	.1092-09	.2157-09	.8128-09	.1959-08

System: C-H-N-O-S-Cl-K-Na-Pb

APPENDIX B

PARTIAL PRESSURES OF GASEOUS TRACE COMPOUNDS PRODUCED AT 1200 K FOR HIGH COAL-HIGH DOLOMITE AND MEAN COAL-LOW DOLOMITE SYSTEMS OPERATING AT 100 PERCENT EXCESS AIR WITH 90 PERCENT SULFUR REMOVAL

TABLE B1. FLUORINE COMPOUNDS

100 Percent Excess Air - 90 Percent Sulfur Removal - 1200 K				
	High Coal - High Dolomite			
Trace Compounds	15 atm	10 atm	5 atm	1 atm
HF	0.9829-04	0.6553-04	0.3275-04	0.6538-05
KF	0.6007-08	0.6417-08	0.7153-08	0.9019-08
NaF	0.1784-08	0.1906-08	0.2124-08	0.2679-08
	Mean Coal - Low Dolomite			
	15 atm	10 atm	5 atm	1 atm
HF	0.7394-04	0.4929-04	0.2464-04	0.4919-05
KF	0.3724-08	0.4013-08	0.4580-08	0.6253-08
NaF	0.1106-08	0.1192-08	0.1360-08	0.1857-08

System: C-H-N-O-S-Cl-K-Na-F

TABLE B2. BERYLLIUM COMPOUNDS

100 Percent Excess Air - 90 Percent Sulfur Removal - 1200 K				
	High Coal - High Dolomite			
Trace Compounds	15 atm	10 atm	5 atm	1 atm
$BeSO_4(s)$	--	--	--	--
$Be(OH)_2$	0.8651-05	0.5768-05	0.2883-05	0.5766-06
	Mean Coal - Low Dolomite			
	15 atm	10 atm	5 atm	1 atm
$BeSO_4(s)$	--	--	--	--
$Be(OH)_2$	0.6647-05	0.4428-05	0.2214-05	0.4430-06

System: C-H-N-O-S-Cl-K-Na-Be

TABLE B3. MERCURY COMPOUNDS

100 Percent Excess Air - 90 Percent Sulfur Removal - 1200 K				
	High Coal - High Dolomite			
Trace Compound	15 atm	10 atm	5 atm	1 atm
Hg	0.7559-07	0.5085-07	0.2576-07	0.5412-08
HgO	0.3461-08	0.1915-08	0.5322-09	0.5683-10
$HgCl_2$	0.2311-09	0.7934-10	0.8872-11	0.4881-13
	Mean Coal - Low Dolomite			
	15 atm	10 atm	5 atm	1 atm
Hg	0.2652-07	0.1338-07	0.6811-08	0.1827-08
HgO	0.2115-08	0.8714-09	0.3138-09	0.3763-10
$HgCl_2$	0.2711-10	0.7006-11	0.1043-11	0.6750-14

System: C-H-N-O-S-Cl-K-Na-Hg

TABLE B4. LEAD COMPOUNDS

100 Percent Excess Air - 90 Percent Sulfur Removal - 1200 K				
	High Coal - High Dolomite			
Trace Compound	15 atm	10 atm	5 atm	1 atm
$PbCl_4$	0.8867-05	0.5894-05	0.2892-05	0.1122-06
$PbCl_2$	0.2622-07	0.3439-07	0.5932-07	0.9984-07
PbCl	0.9026-10	0.1663-09	0.5379-09	0.5963-08
PbO	0.1265-08	0.2675-08	0.1147-07	0.3746-06
	Mean Coal - Low Dolomite			
	15 atm	10 atm	5 atm	1 atm
$PbCl_4$	0.4183-05	0.2715-05	0.1177-05	0.3432-08
$PbCL_2$	0.6445-07	0.8165-07	0.2766-06	0.1463-07
PbCl	0.5064-09	0.8965-09	0.2456-08	0.1912-08
PbO	0.1621-07	0.3273-07	0.1172-06	0.2629-06

System: C-H-N-O-S-Cl-K-Na-Pb

TABLE C1. THERMOCHEMICAL PROPERTIES OF FLUID-BED COMBUSTION GASES CONTAINING TRACE COMPOUNDS

HIGH COAL-HIGH DOLOMITE 10% EXCESS AIR / 90% S REMOVAL

H/RT

	15.0 ATM	10.0 ATM	5.0 ATM	1.0 ATM
300.0 DEGK	-.316073+02	-.316073+02	-.316073+02	-.316073+02
500.0 DEGK	-.174394+02	-.174393+02	-.174391+02	-.174386+02
700.0 DEGK	-.112993+02	-.112989+02	-.112984+02	-.112979+02
900.0 DEGK	-.784564+01	-.784554+01	-.784534+01	-.784482+01
1000.0 DEGK	-.662383+01	-.662371+01	-.662350+01	-.662312+01
1100.0 DEGK	-.561709+01	-.561703+01	-.561696+01	-.561731+01
1200.0 DEGK	-.477252+01	-.477266+01	-.477317+01	-.477595+01

G = KCAL/MOL•DEG K

	15.0 ATM	10.0 ATM	5.0 ATM	1.0 ATM
300.0 DEGK	-.132668+09	-.133679+09	-.135408+09	-.139423+09
500.0 DEGK	-.170278+09	-.171964+09	-.174845+09	-.181534+09
700.0 DEGK	-.210544+09	-.212901+09	-.216932+09	-.226295+09
900.0 DEGK	-.252807+09	-.255841+09	-.261027+09	-.273067+09
1000.0 DEGK	-.274561+09	-.277932+09	-.283693+09	-.297072+09
1100.0 DEGK	-.296683+09	-.300391+09	-.306730+09	-.321457+09
1200.0 DEGK	-.319151+09	-.323199+09	-.330124+09	-.346230+09

SPECIFIC ENTROPY-JOULES/KG

	15.0 ATM	10.0 ATM	5.0 ATM	1.0 ATM
300.0 DEGK	.596808+04	.608023+04	.627195+04	.671712+04
500.0 DEGK	.650505+04	.661722+04	.680898+04	.725425+04
700.0 DEGK	.688104+04	.699328+04	.718512+04	.763047+04
900.0 DEGK	.717555+04	.728775+04	.747956+04	.792495+04
1000.0 DEGK	.730294+04	.741515+04	.760696+04	.805233+04
1100.0 DEGK	.742025+04	.753244+04	.772423+04	.816945+04
1200.0 DEGK	.752901+04	.764116+04	.783281+04	.827733+04

ENTHALPY-JOULE/KG

	15.0 ATM	10.0 ATM	5.0 ATM	1.0 ATM
300.0 DEGK	-.262316+07	-.262316+07	-.262316+07	-.262316+07
500.0 DEGK	-.241230+07	-.241229+07	-.241228+07	-.241223+07
700.0 DEGK	-.218845+07	-.218840+07	-.218834+07	-.218828+07
900.0 DEGK	-.195383+07	-.195381+07	-.195377+07	-.195367+07
1000.0 DEGK	-.183288+07	-.183285+07	-.183281+07	-.183273+07
1100.0 DEGK	-.170977+07	-.170975+07	-.170974+07	-.170981+07
1200.0 DEGK	-.158474+07	-.158478+07	-.158490+07	-.158558+07

Pages 84 and 85 are blank.

TABLE C1. (Cont'd)

HIGH COAL-HIGH DOLOMITE 10% EXCESS AIR / 90% S REMOVAL

COMPRESSIBILITY FACTOR

	15.0 ATM	10.0 ATM	5.0 ATM	1.0 ATM
300.0 DEGK	.382719+02	.382719+02	.382719+02	.382720+02
500.0 DEGK	.382731+02	.382732+02	.382734+02	.382738+02
700.0 DEGK	.382783+02	.382788+02	.382795+02	.382802+02
900.0 DEGK	.382809+02	.382810+02	.382812+02	.382818+02
1000.0 DEGK	.382818+02	.382819+02	.382822+02	.382828+02
1100.0 DEGK	.382826+02	.382827+02	.382830+02	.382841+02
1200.0 DEGK	.382835+02	.382839+02	.382849+02	.382898+02

DENSITY-KG/M3

	15.0 ATM	10.0 ATM	5.0 ATM	1.0 ATM
300.0 DEGK	.183177+02	.122118+02	.610591+01	.122118+01
500.0 DEGK	.109903+02	.732685+01	.366341+01	.732673+00
700.0 DEGK	.784918+01	.523272+01	.261631+01	.523253+00
900.0 DEGK	.610451+01	.406966+01	.203482+01	.406957+00
1000.0 DEGK	.549393+01	.366260+01	.183129+01	.366253+00
1100.0 DEGK	.499439+01	.332959+01	.166479+01	.332965+00
1200.0 DEGK	.457822+01	.305217+01	.152613+01	.305273+00

CP-JOULE/KG,K

	15.0 ATM	10.0 ATM	5.0 ATM	1.0 ATM
300.0 DEGK	.101900+04	.101902+04	.101905+04	.101907+04
500.0 DEGK	.108801+04	.108804+04	.108811+04	.108855+04
700.0 DEGK	.114880+04	.114833+04	.114748+04	.114639+04
900.0 DEGK	.119776+04	.119788+04	.119809+04	.119838+04
1000.0 DEGK	.122072+04	.122072+04	.122066+04	.122028+04
1100.0 DEGK	.124136+04	.124124+04	.124108+04	.124083+04
1200.0 DEGK	.126064+04	.126061+04	.126061+04	.126135+04

CV-JOULE/KG,K

	15.0 ATM	10.0 ATM	5.0 ATM	1.0 ATM
300.0 DEGK	.742396+03	.742402+03	.742415+03	.742456+03
500.0 DEGK	.811290+03	.811329+03	.811394+03	.811794+03
700.0 DEGK	.871785+03	.871366+03	.870604+03	.869643+03
900.0 DEGK	.920960+03	.921070+03	.921261+03	.921517+03
1000.0 DEGK	.943873+03	.943859+03	.943778+03	.943409+03
1100.0 DEGK	.964490+03	.964439+03	.964295+03	.964073+03
1200.0 DEGK	.983874+03	.983846+03	.983858+03	.984558+03

TABLE C1. (Cont'd)

HIGH COAL-HIGH DOLOMITE 10% EXCESS AIR / 90% S REMOVAL

MOL.WT.-KG/MOLE

	15.0 ATM	10.0 ATM	5.0 ATM	1.0 ATM
300.0 DEGK	.300618+02	.300618+02	.300618+02	.300618+02
500.0 DEGK	.300609+02	.300608+02	.300607+02	.300603+02
700.0 DEGK	.300569+02	.300565+02	.300560+02	.300554+02
900.0 DEGK	.300549+02	.300548+02	.300546+02	.300542+02
1000.0 DEGK	.300542+02	.300541+02	.300539+02	.300535+02
1100.0 DEGK	.300537+02	.300536+02	.300535+02	.300541+02
1200.0 DEGK	.300538+02	.300541+02	.300550+02	.300596+02

TOTAL MOLES

	15.0 ATM	10.0 ATM	5.0 ATM	1.0 ATM
300.0 DEGK	.382719+02	.382719+02	.382719+02	.382720+02
500.0 DEGK	.382731+02	.382732+02	.382734+02	.382738+02
700.0 DEGK	.382783+02	.382788+02	.382795+02	.382802+02
900.0 DEGK	.382809+02	.382810+02	.382812+02	.382818+02
1000.0 DEGK	.382818+02	.382819+02	.382822+02	.382828+02
1100.0 DEGK	.382826+02	.382827+02	.382830+02	.382841+02
1200.0 DEGK	.382835+02	.382839+02	.382849+02	.382898+02

MASS-KG

	15.0 ATM	10.0 ATM	5.0 ATM	1.0 ATM
300.0 DEGK	.115052+01	.115052+01	.115052+01	.115052+01
500.0 DEGK	.115052+01	.115052+01	.115052+01	.115052+01
700.0 DEGK	.115053+01	.115053+01	.115053+01	.115053+01
900.0 DEGK	.115053+01	.115053+01	.115053+01	.115053+01
1000.0 DEGK	.115053+01	.115053+01	.115053+01	.115053+01
1100.0 DEGK	.115053+01	.115053+01	.115054+01	.115060+01
1200.0 DEGK	.115057+01	.115059+01	.115065+01	.115098+01

FLUX-WATTS/CM2.ATM

	15.0 ATM	10.0 ATM	5.0 ATM	1.0 ATM
300.0 DEGK	-.108104+06	-.108105+06	-.108105+06	-.108104+06
500.0 DEGK	-.761158+05	-.761149+05	-.761135+05	-.761084+05
700.0 DEGK	-.578457+05	-.578462+05	-.578485+05	-.578510+05
900.0 DEGK	-.452468+05	-.452458+05	-.452440+05	-.452405+05
1000.0 DEGK	-.401548+05	-.401545+05	-.401541+05	-.401536+05
1100.0 DEGK	-.356278+05	-.356266+05	-.356267+05	-.356291+05
1200.0 DEGK	-.315460+05	-.315469+05	-.315497+05	-.315635+05

TABLE C1. (Cont'd)

HIGH COAL-HIGH DOLOMITE 10% EXCESS AIR / 90% S REMOVAL

GAMMA

	15.0 ATM	10.0 ATM	5.0 ATM	1.0 ATM
300.0 DEGK	.137259+01	.137259+01	.137261+01	.137257+01
500.0 DEGK	.134107+01	.134105+01	.134103+01	.134091+01
700.0 DEGK	.131771+01	.131781+01	.131801+01	.131823+01
900.0 DEGK	.130055+01	.130052+01	.130048+01	.130043+01
1000.0 DEGK	.129329+01	.129332+01	.129337+01	.129347+01
1100.0 DEGK	.128705+01	.128699+01	.128702+01	.128706+01
1200.0 DEGK	.128130+01	.128130+01	.128129+01	.128111+01

ACOUSTIC VELOCITY-M/SEC

	15.0 ATM	10.0 ATM	5.0 ATM	1.0 ATM
300.0 DEGK	.337472+03	.337473+03	.337475+03	.337471+03
500.0 DEGK	.430651+03	.430648+03	.430645+03	.430629+03
700.0 DEGK	.505129+03	.505151+03	.505193+03	.505240+03
900.0 DEGK	.569039+03	.569034+03	.569026+03	.569020+03
1000.0 DEGK	.598151+03	.598158+03	.598171+03	.598198+03
1100.0 DEGK	.625836+03	.625823+03	.625831+03	.625833+03
1200.0 DEGK	.652199+03	.652197+03	.652185+03	.652091+03